Transformer Models

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Attention Is All You Need (Google)

Transformer (Google 2017)

- Transformer was developed for solving text translation problem.

- The Transformer architecture consists of an Encoder and a Decoder and the Encoder’s output is an input to the Decoder.

Attention Is All You Need

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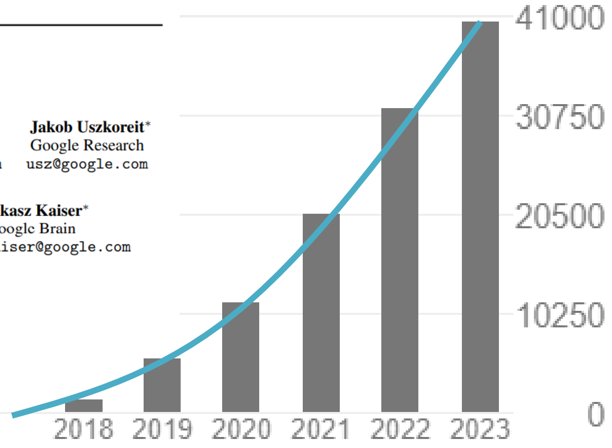
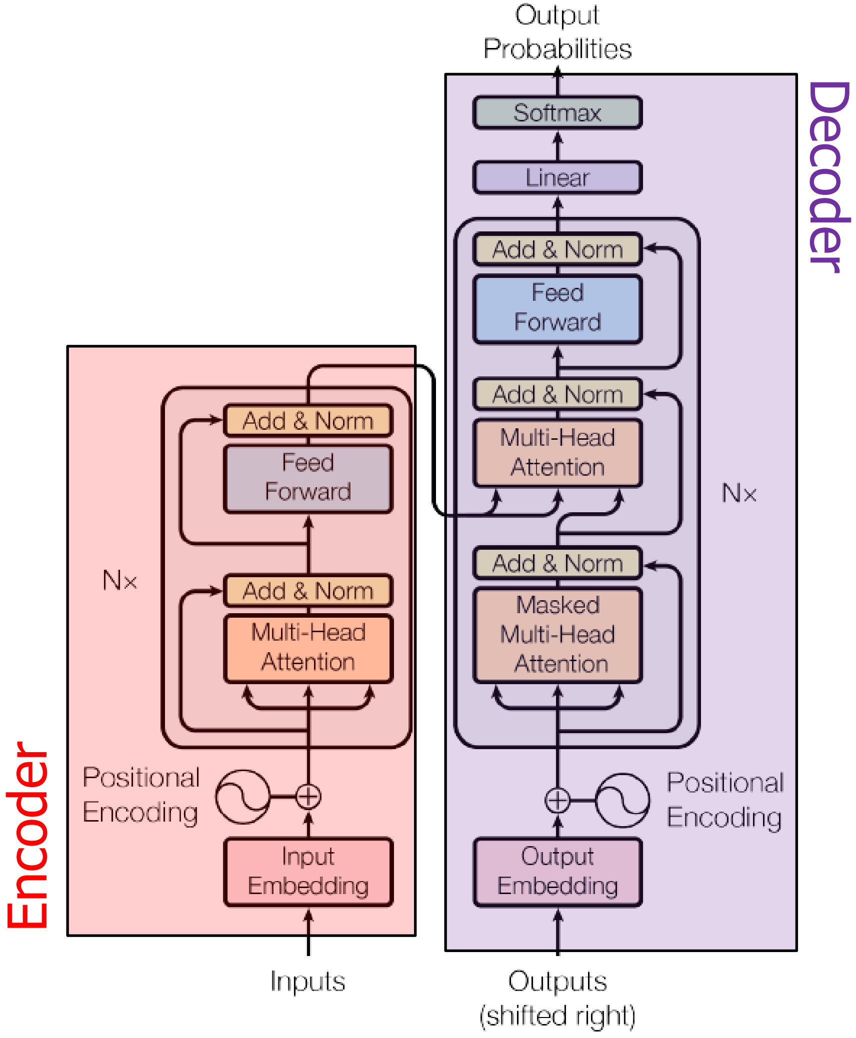
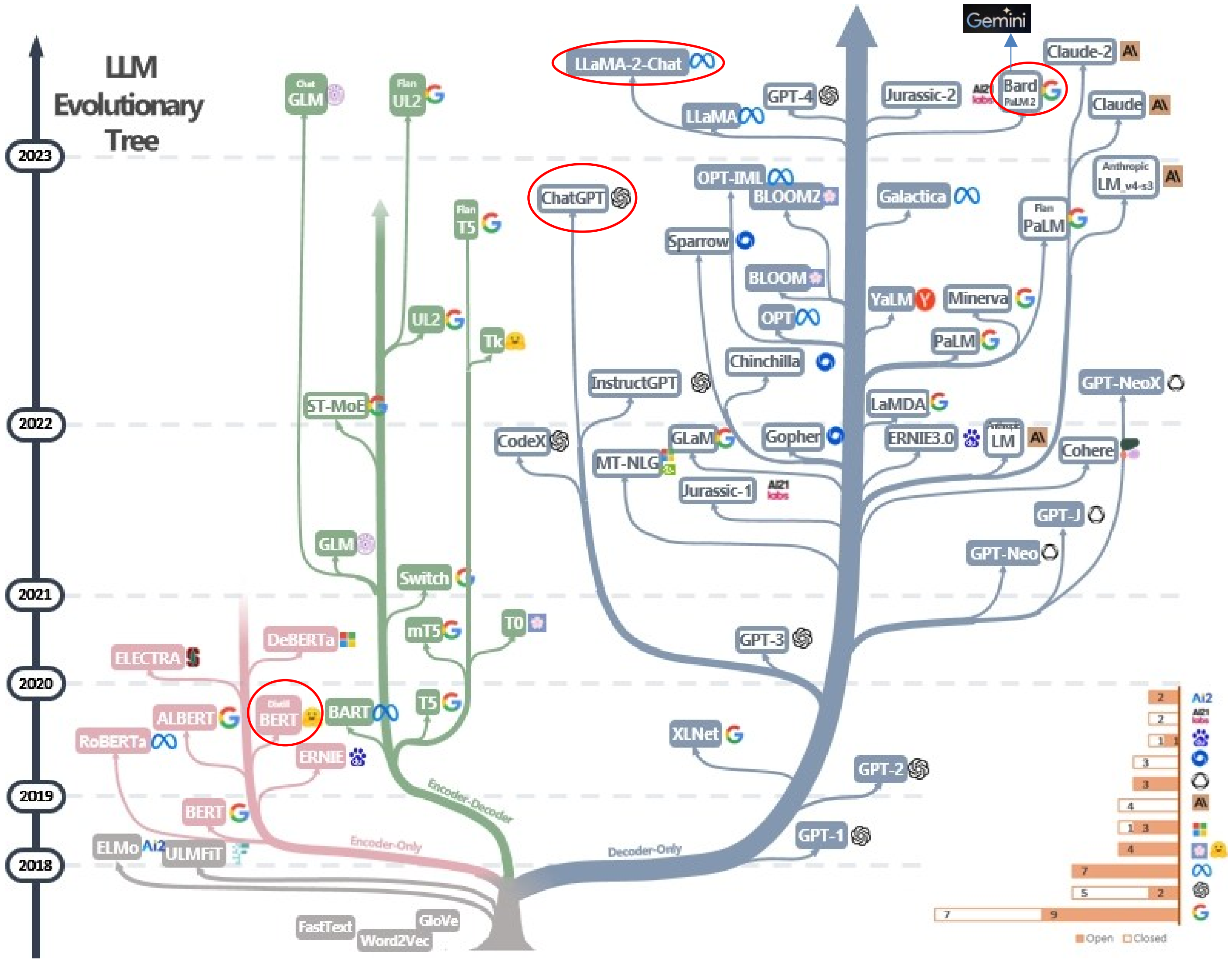




LLM Evolutionary Tree



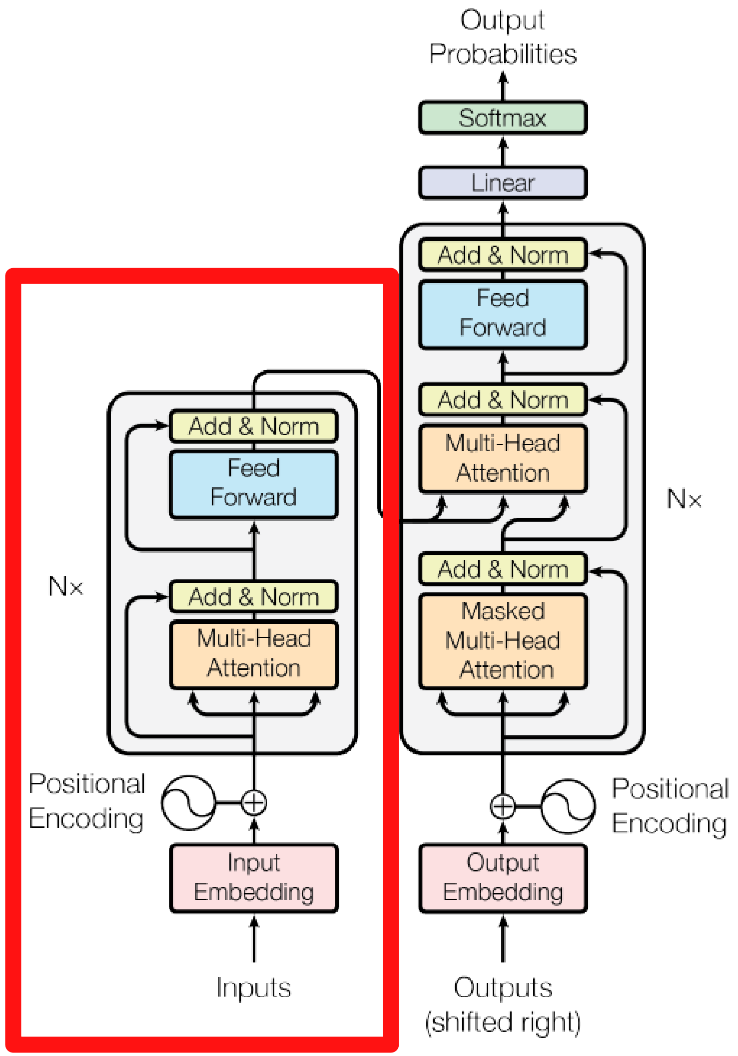
BERT: Bidirectional Encoder Representations from Transformers

BERT (Google 2018)

- BERT is a paper published by researchers at Google AI Language.
- It has caused a stir in the Machine Learning community by presenting state-of-the-art results in a wide variety of NLP tasks:
    - Question Answering (SQuAD v2.0);
    - Named Entity Recognition
- BERT's key technical innovation is applying the bidirectional training of Transformer, a popular attention model, to language modelling.
- This is in contrast to previous efforts which looked at a text sequence either from left to right or combined left-to-right and right-to-left training.
- The paper's results show that a language model which is bidirectionally trained can have a deeper sense of language context and flow than single-direction language models.

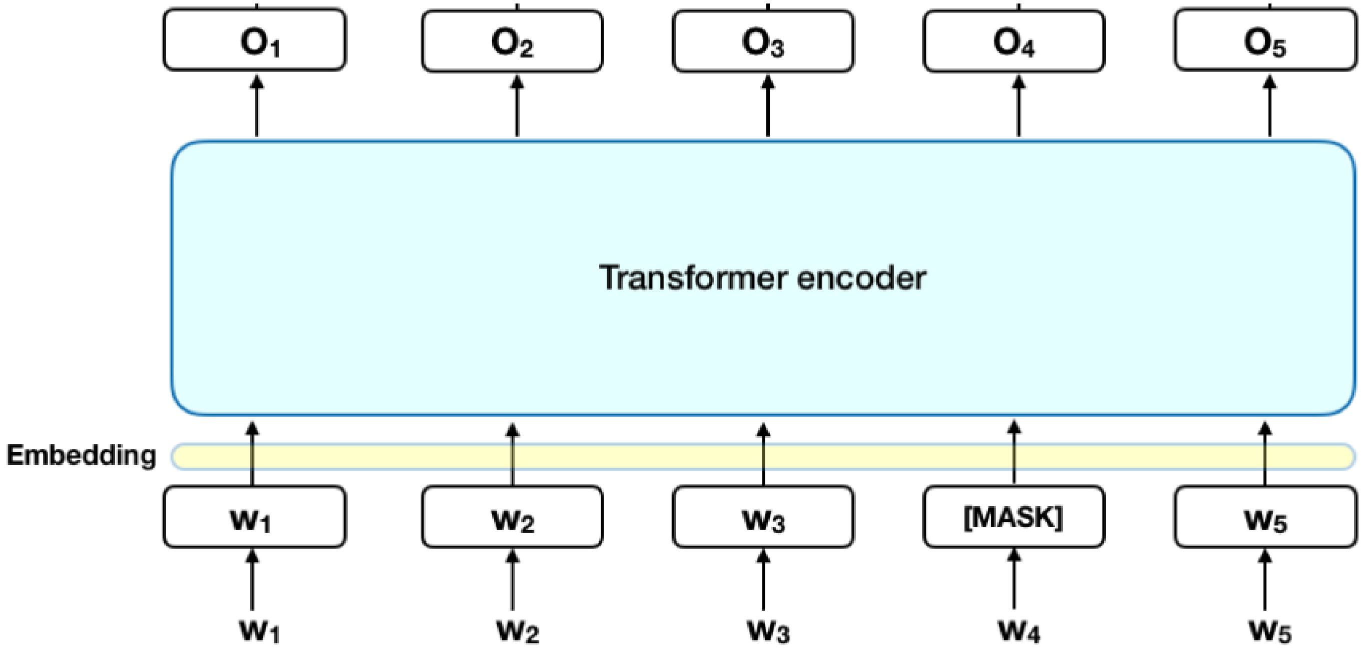
BERT (Google 2018)

- In short BERT consists of the Encoder, introduced in the paper Attention Is All You Need, with some novel modifications.



Transformer Encoder

- The input is a sequence of tokens, which are first embedded into vectors and then processed in the neural network.
- The output is a sequence of vectors of size H, in which each vector corresponds to an input token with the same index.



Information Flow

The data flow through the architecture is as follows:

1. The model represents each token as a vector of emb_dim size. We have a matrix of dimensions (input_length) x (emb_dim) for a specific input sequence.

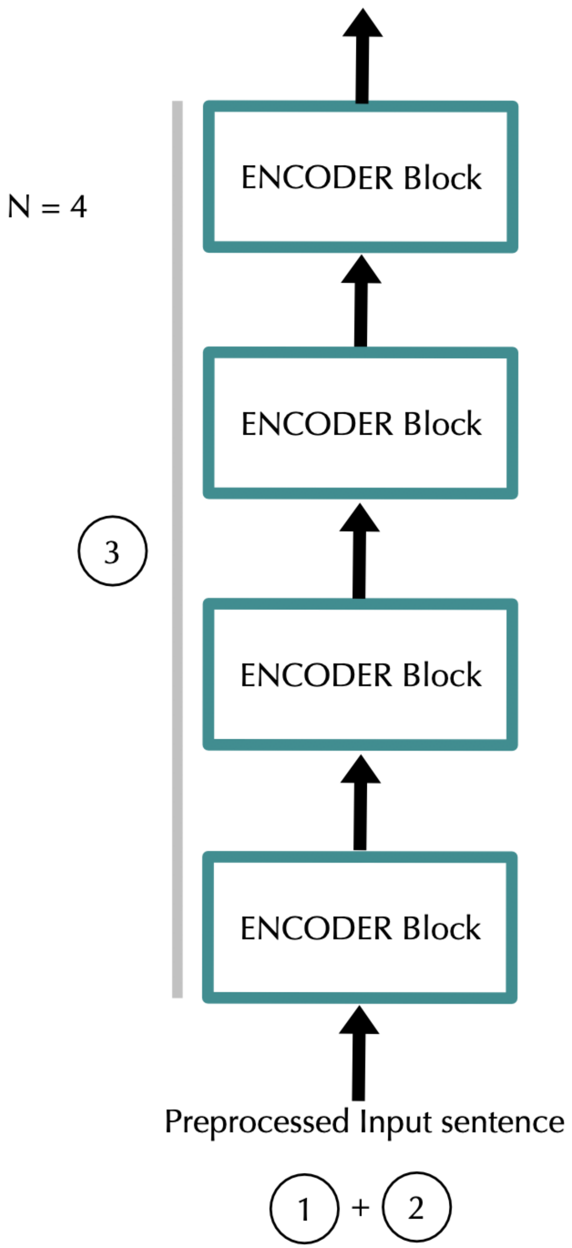
2. It then adds positional information (positional encoding). Matrix of dimensions remains the same.

3. The data goes through N encoder blocks. After this, we obtain the same matrix dimensions

Note:

- In the Bert's experiments, they use N=12 or 24

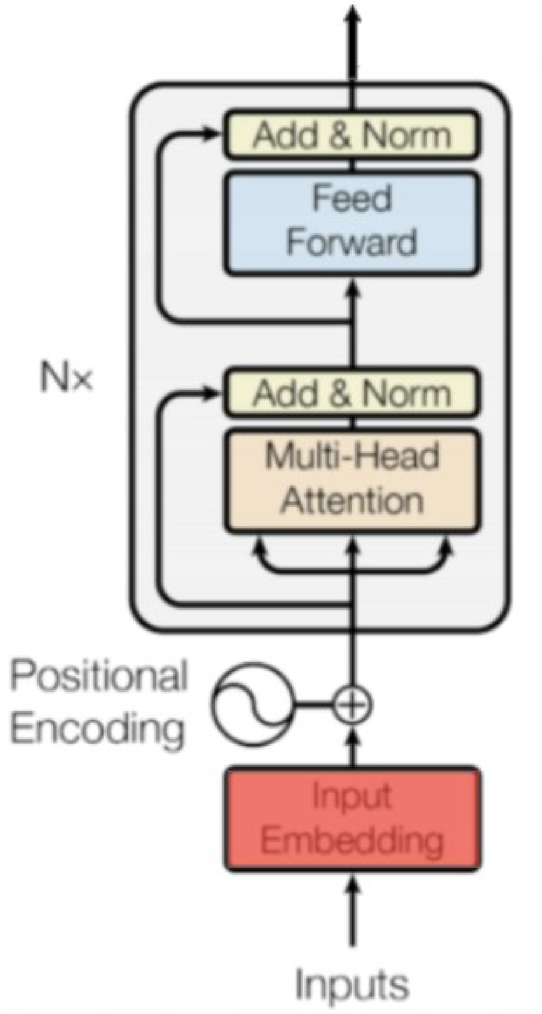
- The blocks do not share weights



From Words to Vectors

From Words to Vectors: Tokenization, numericalization and word embeddings

- Tokenization, numericalization and embeddings do not differ from the way it is done with RNNs.
- Given a sentence in a corpus:
- " Hello, how are you?"
- The first step is to tokenize it:
- " Hello, how are you?" → ["Hello", "," , "how", "are", "you", "?"]



From Words to Vectors

1. This is followed by numericalization, mapping each token to a unique integer in the corpus' vocabulary.

2. ["Hello", ", ", "how", "are", "you", "?"] → [34, 90, 15, 684, 55, 193]

3. Next, we get the embedding for each word in the sequence.

4. Each word of the sequence is mapped to an emb_dim dimensional vector that the model will learn during training.

5. The elements of those vectors are treated as model parameters and are optimized with back-propagation just like any other weights.

From Words to Vectors

- For each token, we look up the corresponding vector:

$$34 \rightarrow E[34] = [123.4, 0.32, \cdots, 94, 32]$$
$$90 \rightarrow E[90] = [83, 34, \cdots, 77, 19]$$
$$15 \rightarrow E[15] = [0.2, 50, \cdots, 33, 30]$$
$$684 \rightarrow E[684] = [289, 432.98, \cdots, 150, 92]$$
$$55 \rightarrow E[55] = [80, 46, \cdots, 23, 32]$$
$$193 \rightarrow E[193] = [41, 21, \cdots, 74, 33]$$

From Words to Vectors

- Stacking each of the vectors together we obtain a matrix Z of dimensions (input_length) x (emb_dim) :

$$\begin{array}{cc} & \begin{matrix} < & \quad - \quad & d_{emb\_dim} & \quad - \quad & > \end{matrix} \\ \begin{matrix} Hello \\ , \\ how \\ are \\ you \\ ? \end{matrix} & \begin{pmatrix} 123.4 & 0.32 & \cdots & 94 & 32 \\ 83 & 34 & \cdots & 77 & 19 \\ 0.2 & 50 & \cdots & 33 & 30 \\ 289 & 432.98 & \cdots & 150 & 92 \\ 80 & 46 & \cdots & 23 & 32 \\ 41 & 21 & \cdots & 74 & 33 \end{pmatrix} \end{array}$$

Padding

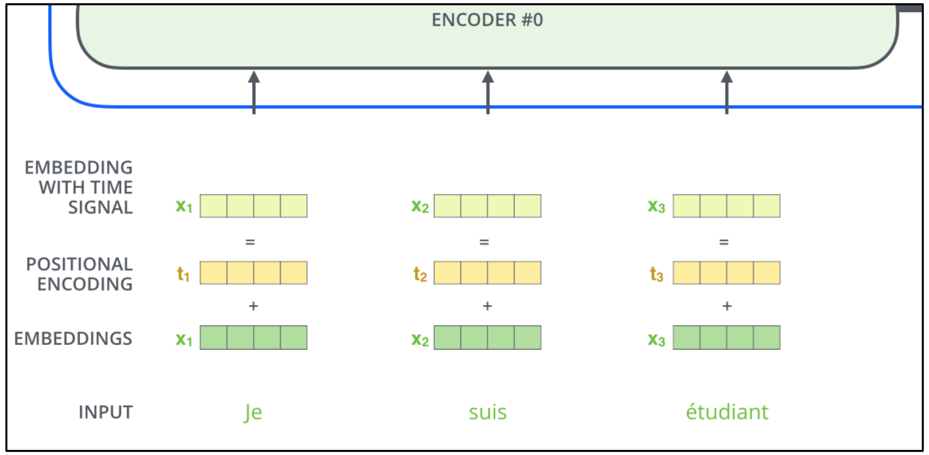
- It is important to remark that padding was used to make the input sequences in a batch have the same length.

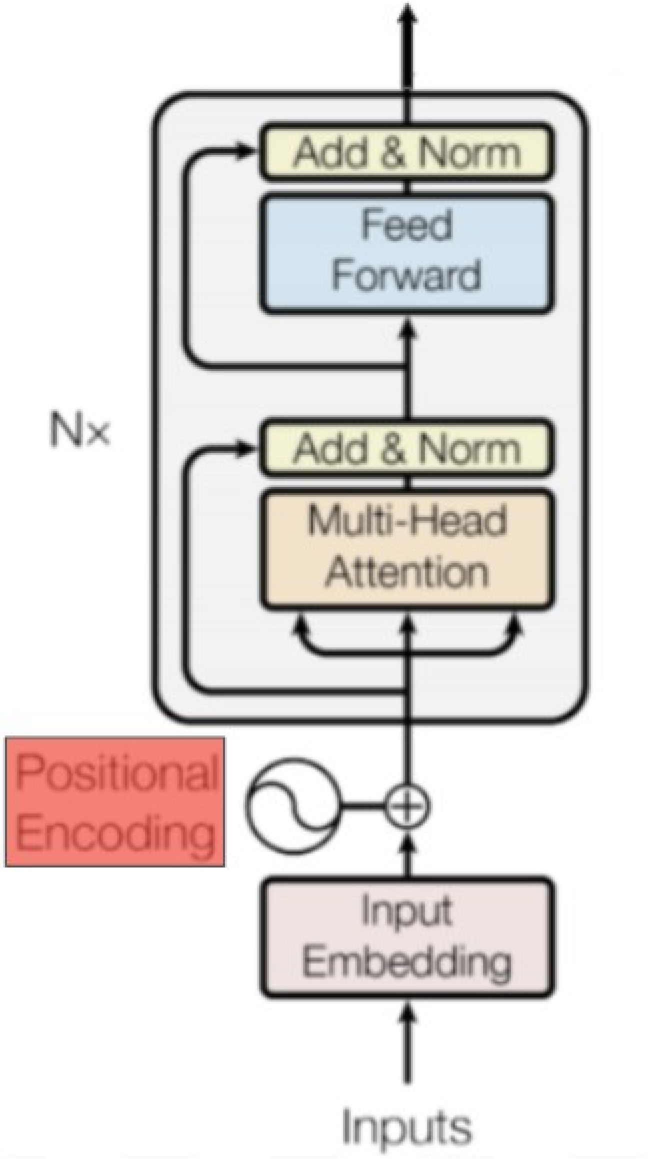
- [“<pad>”, “<pad>”, “<pad>”, “Hello”, “, “, “how”, “are”, “you”, “?”] →

- [5, 5, 5, 34, 90, 15, 684, 55, 193]

Positional Encoding

- In BERT the authors used learned positional embeddings.
- At the beginning they add a random numbers



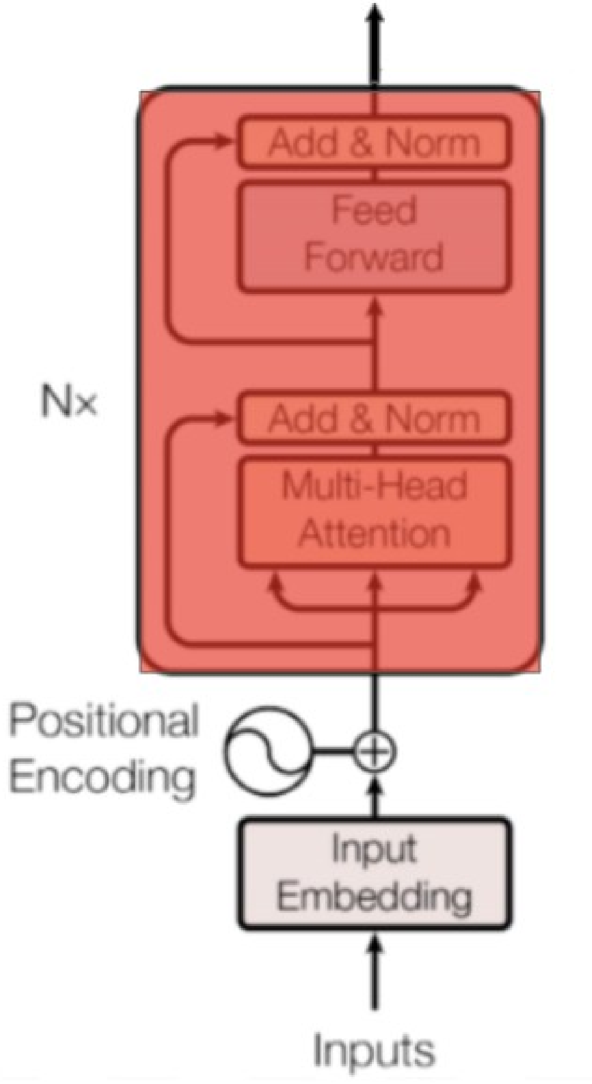


Encoder block

- **A total of N encoder blocks are chained together** to generate the Encoder's output.

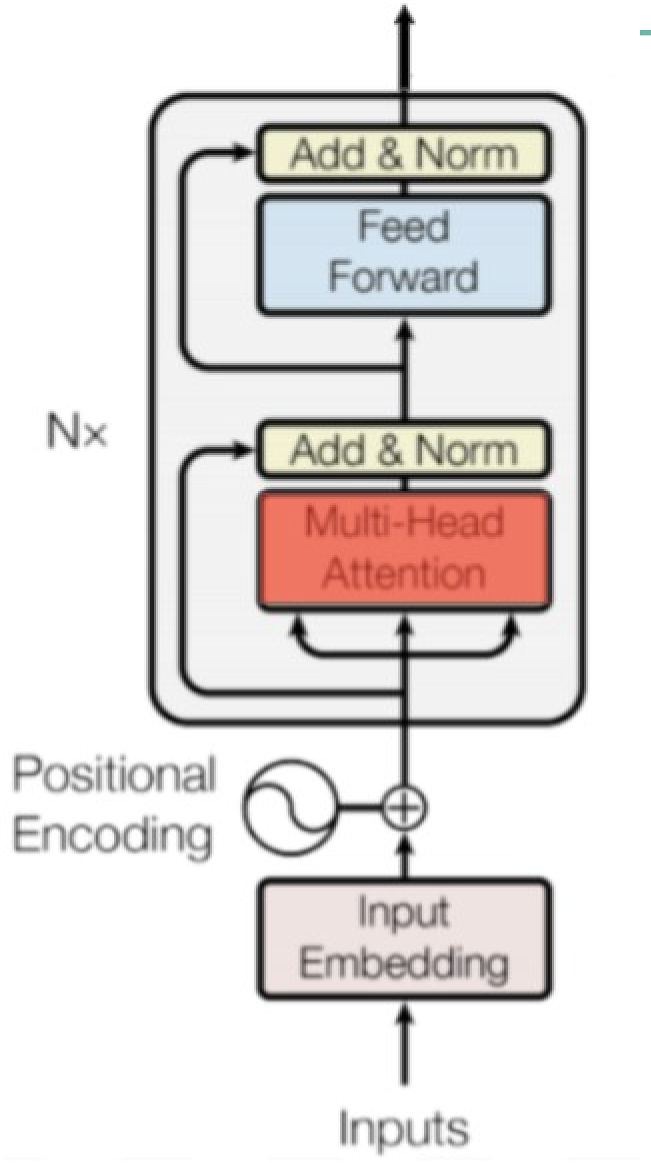
- A **specific block** is in charge of **finding relationships** between the input representations and encode them in its output.

- This **iterative process** through the blocks will help the **neural network to capture more complex relationships between words in the input sequence**.



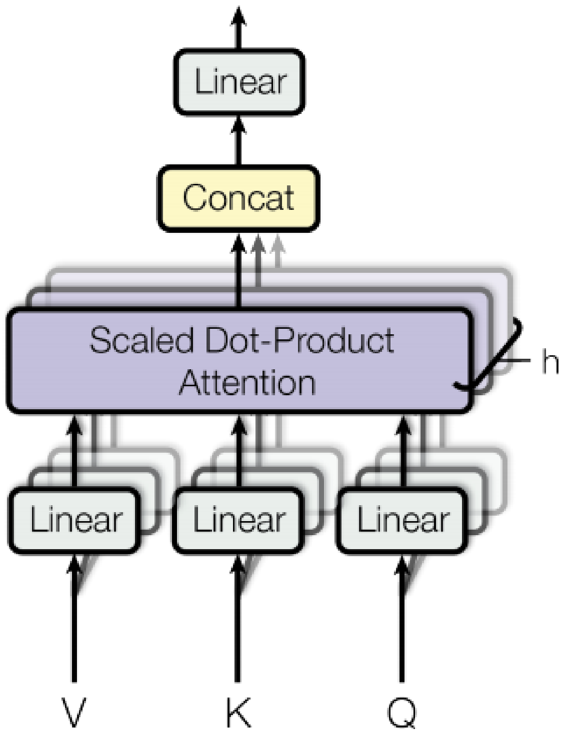
Multi-Head Attention

- The Transformer uses Multi-Head Attention, which means it computes **attention h different times** with different weight matrices and then concatenates the results together.



Multi-Head Attention

- The result of each of those parallel computations of attention is called a head.

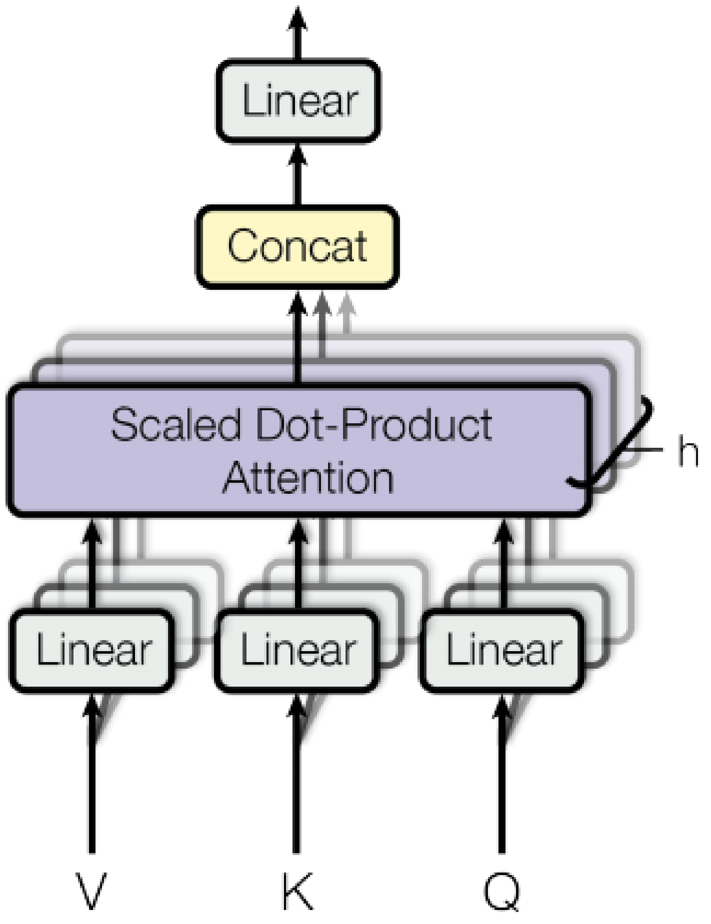


$$\mathrm{MultiHead}(Q, K, V) = \mathrm{Concat}(\mathrm{head_1}, ..., \mathrm{head_h})W^O$$
$$\text{where } \mathrm{head_i} = \mathrm{Attention}(QW_i^Q, KW_i^K, VW_i^V)$$

Multi-Head Attention

- Let's

$$VW_i^V = V_i$$
$$KW_i^K = K_i$$
$$QW_i^Q = Q_i$$



Scaled Dot-Product Attention

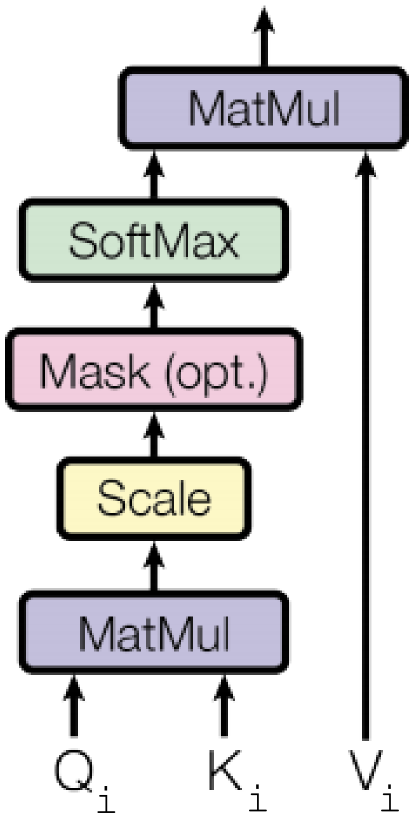
$$\mathrm{Attention}(Q, K, V) = \mathrm{softmax}(\frac{QK^T}{\sqrt{d_k}})V$$

- Let's start by looking at the matrix product between Q_i and K_i transposed:

$$Q_i K_i^T$$

- Remember Q_i and K_i are different projections of the tokens into another dimensional space (d_k).

- Therefore, **we can think about the dot product of those projections as a measure of similarity between tokens projections**.

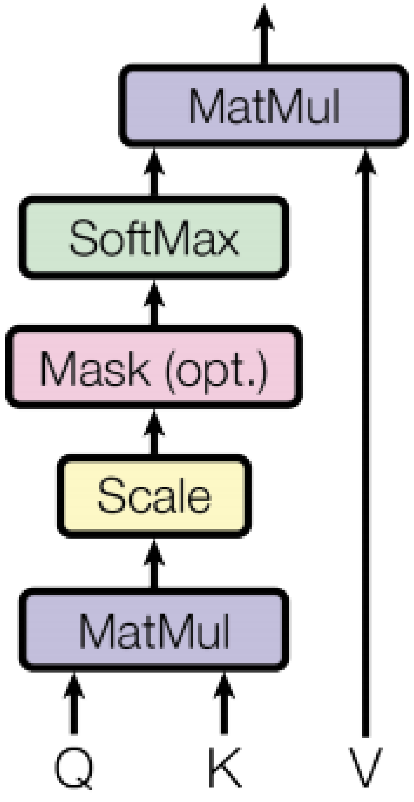


Scaled Dot-Product Attention

- If we call v_i and u_j the projections of the i-th token and the j-th token through Q_i and K_i respectively, their dot product can be seen as:

$$v_i u_j = \cos(v_i, u_j)||v_i||_2||u_j||_2$$

- Thus, this is a **measure of how similar** are the **directions** of $\boldsymbol{v_i}$ and $\boldsymbol{u_j}$ and how large are their **lengths** (the closest the direction and the larger the length, the greater the dot product)



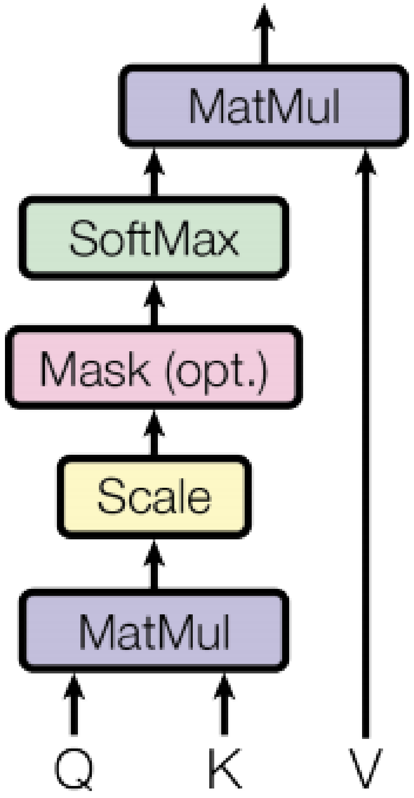
Scaled Dot-Product Attention

- After this multiplication, the **matrix is divided element-wise** by the square root of d_k for **scaling purposes**.

- **Mask Layer deals with Padding tokens**

- The next step is a **Softmax applied row-wise (one softmax computation for each row)**:

$$Softmax\left(\frac{Q_i K_i^T}{\sqrt{d_k}}\right)$$



Softmax (Example)

- Before Softmax

$$
\begin{array}{cc}
 & \begin{array}{cccccc} Hello & , & how & are & you & ? \end{array} \\
\begin{array}{c} Hello \\ , \\ how \\ are \\ you \\ ? \end{array} &
\begin{pmatrix}
78.49 & 43.29 & 1.2 & 41.74 & 91.43 & 74.47 \\
95.84 & 28.78 & 57.13 & 68.20 & -60.94 & 26.85 \\
-95.69 & -52.16 & 17.00 & 45.71 & 48.49 & 64.35 \\
-69.92 & 85.16 & 94.94 & 91.04 & -92.83 & 77.49 \\
65.85 & 55.85 & 62.54 & -97.46 & 76.38 & 13.20 \\
-30.05 & -4.52 & 76.02 & 42.35 & 15.29 & 63.61
\end{pmatrix}
\end{array}
\Longrightarrow
$$

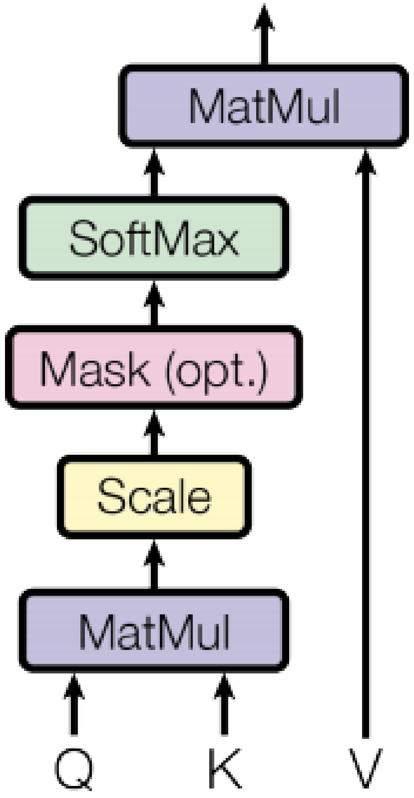
- After Softmax

$$
\begin{array}{ccc}
 & \begin{array}{cccccc} Hello & , & how & are & you & ? \end{array} & \\
\begin{array}{c} Hello \\ , \\ how \\ are \\ you \\ ? \end{array} &
\begin{pmatrix}
72.40 * 10^{-06} & 1.23 * 10^{-21} & 6.51 * 10^{-40} & 2.62 * 10^{-22} & 9.99 * 10^{-01} & 4.30 * 10^{-08} \\
1.00 * 10^{+00} & 7.51 * 10^{-30} & 1.54 * 10^{-17} & 9.91 * 10^{-13} & 8.15 * 10^{-69} & 1.09 * 10^{-30} \\
3.12 * 10^{-70} & 2.51 * 10^{-51} & 2.72 * 10^{-21} & 8.03 * 10^{-09} & 1.29 * 10^{-07} & 9.99 * 10^{-01} \\
2.47 * 10^{-72} & 5.54 * 10^{-05} & 9.80 * 10^{-01} & 1.98 * 10^{-02} & 2.77 * 10^{-82} & 2.58 * 10^{-08} \\
2.67 * 10^{-05} & 1.21 * 10^{-09} & 9.75 * 10^{-07} & 3.17 * 10^{-76} & 9.99 * 10^{-01} & 3.64 * 10^{-28} \\
8.59 * 10^{-47} & 1.05 * 10^{-35} & 9.99 * 10^{-01} & 2.38 * 10^{-15} & 4.21 * 10^{-27} & 4.07 * 10^{-06}
\end{pmatrix} &
\begin{array}{c} = 1 \\ = 1 \\ = 1 \\ = 1 \\ = 1 \\ = 1 \end{array}
\end{array}
$$

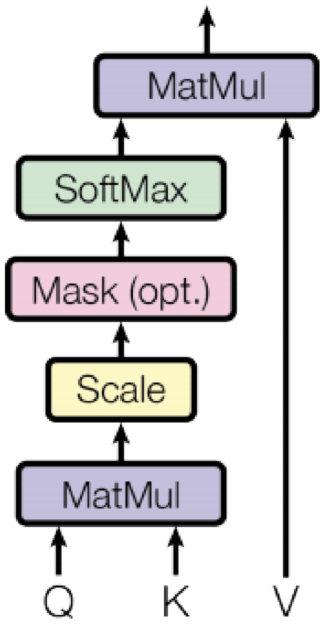
Scaled Dot-Product Attention

- The result would be rows with numbers between zero and one that sum to one. Finally, the result is multiplied by V_i to get the result of the head.

$$Softmax\left(\frac{Q_i K_i^T}{\sqrt{d_k}}\right) V_i$$



Example #1



- Let's propose a dummy example. Suppose that the resulting first row of:

$$Softmax\left(\frac{Q_i K_i^T}{\sqrt{d_k}}\right)$$

- is [0,0,0,0,1,0]. So:

$$\begin{array}{c} \\ Hello \\ , \\ how \\ are \\ you \\ ? \end{array}
\begin{array}{c} \begin{array}{cccccc} Hello & , & how & are & you & ? \end{array} \\ \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} \end{array}
\begin{array}{c} d_v \\ \begin{pmatrix} v_{Hello} \\ v_{,} \\ v_{how} \\ v_{are} \\ v_{you} \\ v_{?} \end{pmatrix} \end{array}
=
\begin{array}{c} \\ Hello \\ , \\ how \\ are \\ you \\ ? \end{array}
\begin{array}{c} d_v \\ \begin{pmatrix} v_{you} \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ \cdots \end{pmatrix} \end{array}$$

Example #1

$$
\begin{array}{c}
 \\ Hello \\ , \\ how \\ are \\ you \\ ?
\end{array}
\begin{array}{c}
\begin{array}{cccccc} Hello & , & how & are & you & ? \end{array} \\
\begin{pmatrix}
0 & 0 & 0 & 0 & 1 & 0 \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots
\end{pmatrix}
\end{array}
\begin{array}{c}
d_v \\
\begin{pmatrix} v_{Hello} \\ v_{,} \\ v_{how} \\ v_{are} \\ v_{you} \\ v_{?} \end{pmatrix}
\end{array}
=
\begin{array}{c}
 \\ Hello \\ , \\ how \\ are \\ you \\ ?
\end{array}
\begin{array}{c}
d_v \\
\begin{pmatrix} v_{you} \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ \cdots \end{pmatrix}
\end{array}
$$

- Observe that in this case the **word "hello" ends up with a representation** based on the 5th token **"you" of the input for that head**.

- Supposing an equivalent example for the rest of the heads. **The word "Hello" will be now represented by the concatenation of the different projections of other words**.

- **The network will learn over training time which relationships are more useful and will relate tokens to each other based on these relationships.**

Example #2

- Let us now complicate the example a little bit more.

$$
\begin{array}{c|cccccc|}
 & Hello & , & how & are & you & ? \\
\hline
Hello & 0.1 & 0 & 0.06 & 0.1 & 0.6 & 0.14 \\
, & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
how & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
are & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
you & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
? & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots
\end{array}
\begin{array}{c}
d_v \\
\begin{pmatrix} v_{Hello} \\ v_{,} \\ v_{how} \\ v_{are} \\ v_{you} \\ v_{?} \end{pmatrix}
\end{array} =
$$

- This results in

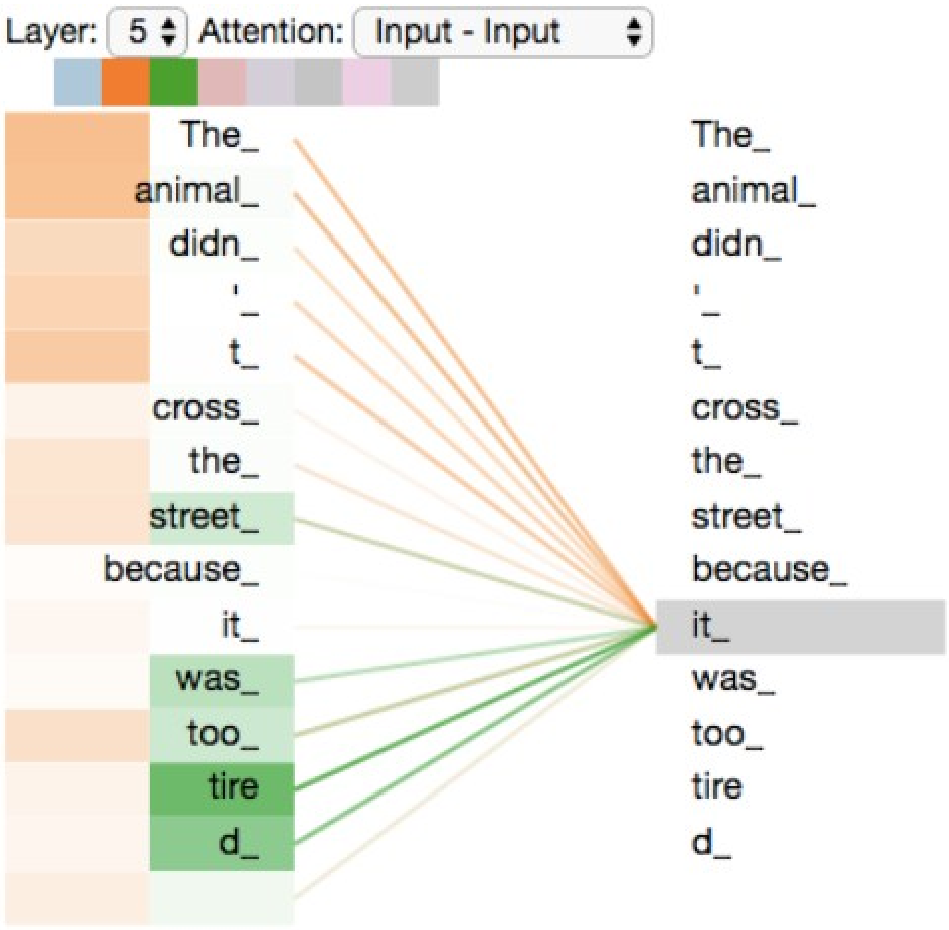
$$
\begin{array}{cc}
 & <-------------d_v------------> \\
\begin{array}{c} Hello \\ , \\ how \\ are \\ you \\ ? \end{array} &
\begin{pmatrix}
0.1v_{Hello} + 0v_{,} + 0.06v_{how} + 0.1v_{are} + 0.6v_{you} + 0.14v_{?} \\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots
\end{pmatrix}
\end{array}
$$

Example #2

$$
\begin{array}{c c}
 & <-\,-\,-\,-\,-\,-\,-\,-\,-\,-\,-\,-\,-\,-\,- \; d_v \; -\,-\,-\,-\,-\,-\,-\,-\,-\,-\,-\,-\,-\,-\,-> \\
\begin{array}{c} Hello \\ , \\ how \\ are \\ you \\ ? \end{array} &
\begin{pmatrix}
0.1v_{Hello} + 0v_{,} + 0.06v_{how} + 0.1v_{are} + 0.6v_{you} + 0.14v_{?} \\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots
\end{pmatrix}
\end{array}
$$

- Observe that we can think about the resulting **representation of “Hello”** as **a weighted combination (centroid) of the projected vectors through V_i of the input tokens**.

Example #3


Layer: 5 Attention: Input - Input
The_
animal_
didn_
'_
t_
cross_
the_
street_
because_
it_
was_
too_
tire
d_
The_
animal_
didn_
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t_
cross_
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street_
because_
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was_
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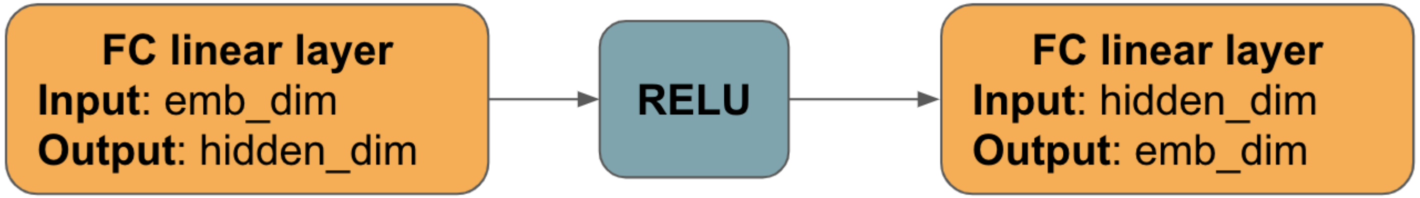
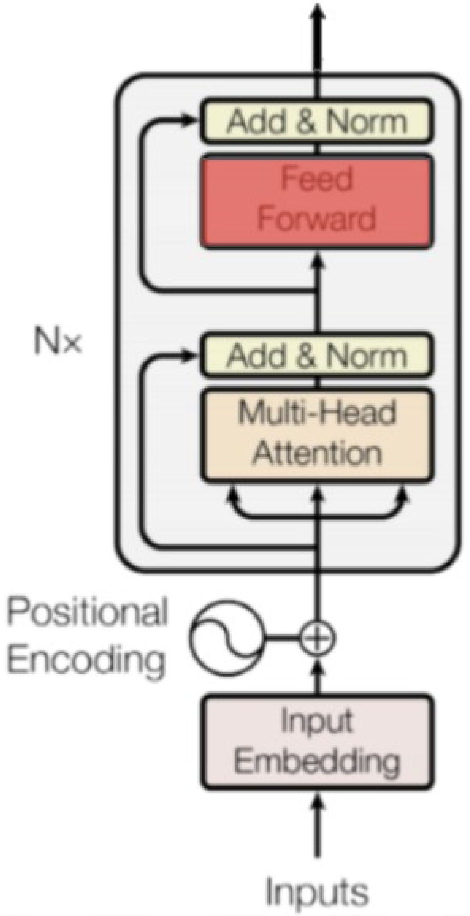
tire
d_

Position-wise Feed-Forward Network

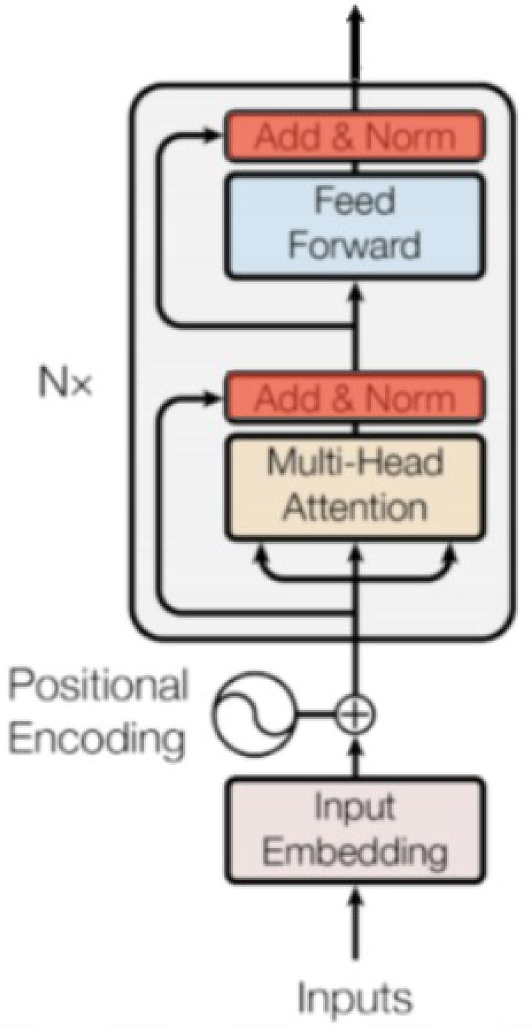
- This step is composed of the following layers:





Dropout, Add & Norm

- In this layer is applied a dropout at 10% in the input.
- This result is added to the original input.
- It is like telling the token:
- **"Learn the relationship with the rest of the tokens, but don't forget what we already learned about yourself!"**
- A token-wise/row-wise normalization is computed with the mean and standard deviation of each row (improves the stability of the network).
- The output of these layers is: $LayerNorm(x + Dropout(Sublayer(x)))$

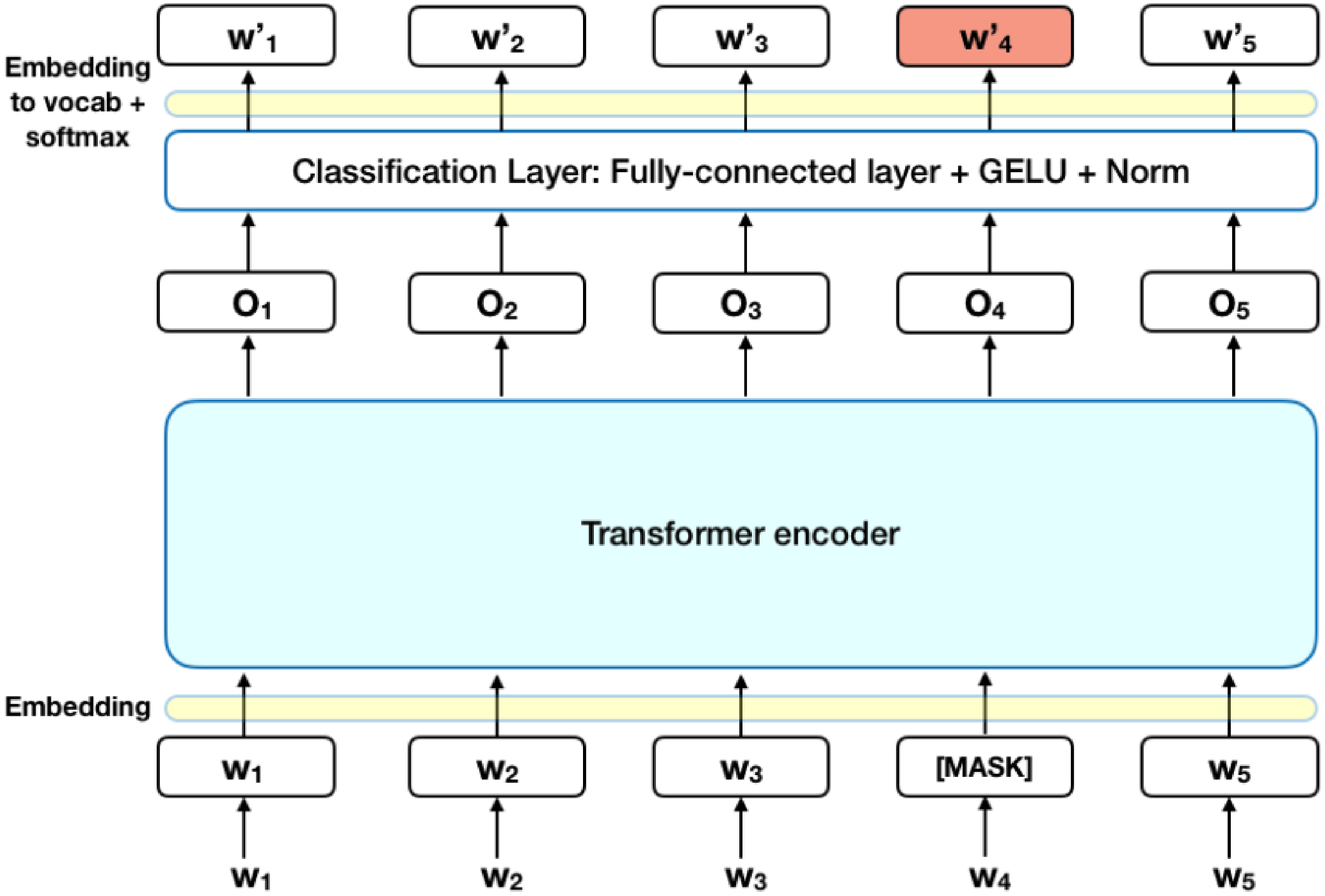


BERT'S TRAINING

BERT'S TRAINING

- When training language models, there is a challenge of defining a prediction goal.
- Many models predict the next word in a sequence (e.g. "The child came home from ___"), a directional approach which inherently limits context learning.
- To overcome this challenge, BERT uses two training strategies simultaneously: Masked Language Model and Next Sentence Prediction.

Task1: Masked Language Model



Task1: Masked Language Model

- The **Masked Language Model asks the model to predict**, not the next word for a sequence of words, but rather **random words from within the sequence**.

- In technical terms, the prediction of the output words requires:

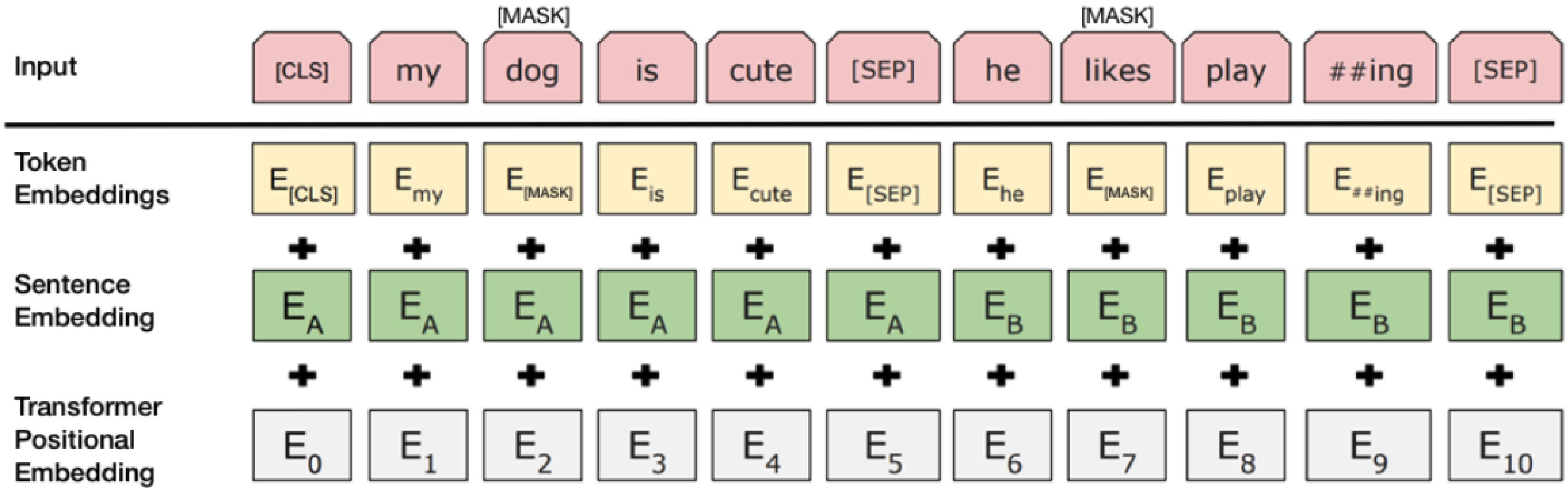
  - Adding a **classification layer** on top of the encoder output.

  - **Multiplying the output vectors by the embedding matrix**, transforming them into the vocabulary dimension.

  - **Calculating the probability of each word in the vocabulary with softmax**.

- Note: Before feeding word sequences into BERT, 15% of the words in each sequence are replaced with a [MASK] token.

Task 2: Next Sentence Prediction



Task 2: Next Sentence Prediction

- This task consists of giving the model two sentences and asking it to predict if the second sentence follows the first in a corpus or not.

- To help the model distinguish between the two sentences in training, the input is processed in the following way before entering the model:

  - A [CLS] token is inserted at the beginning of the first sentence and a [SEP] token is inserted at the end of each sentence.

  - A sentence embedding indicating Sentence A or Sentence B is added to each token.

  - A positional embedding is added to each token to indicate its position in the sequence.

- During training, 50% of the inputs are a pair in which the second sentence is the subsequent sentence in the original document, while in the other 50% a random sentence from the corpus is chosen as the second sentence.

Task 2: Next Sentence Prediction

- To predict if the second sentence is indeed connected to the first, the following steps are performed:
  - The entire input sequence goes through the Transformer model.
  - The output of the [CLS] token is transformed into a 2×1 shaped vector, using a simple classification layer (learned matrices of weights and biases).
  - Calculating the probability of IsNextSequence with softmax.

Fine-tuning

Fine-tuning

- **BER**T can be used for a **wide variety of language tasks**, while only adding a small layer to the core model:

1. **Classification tasks** such as sentiment analysis are done similarly to **Next Sentence classification**, by adding a classification layer on top of the Transformer output for the [CLS] token.

2. In **Question Answering tasks** (e.g. SQuAD v2.0), the software receives a question regarding a text sequence and is required to mark the answer in the sequence. Using BERT, a Q&A model can be trained by learning **two extra vectors that mark the beginning and the end of the answer**.

3. In **Named Entity Recognition** (NER), the software receives a text sequence and is required to mark the various types of entities (Person, Organization, Date, etc) that appear in the text. Using BERT, a NER model **can be trained by feeding the output vector of each token into a classification layer that predicts the NER label**.

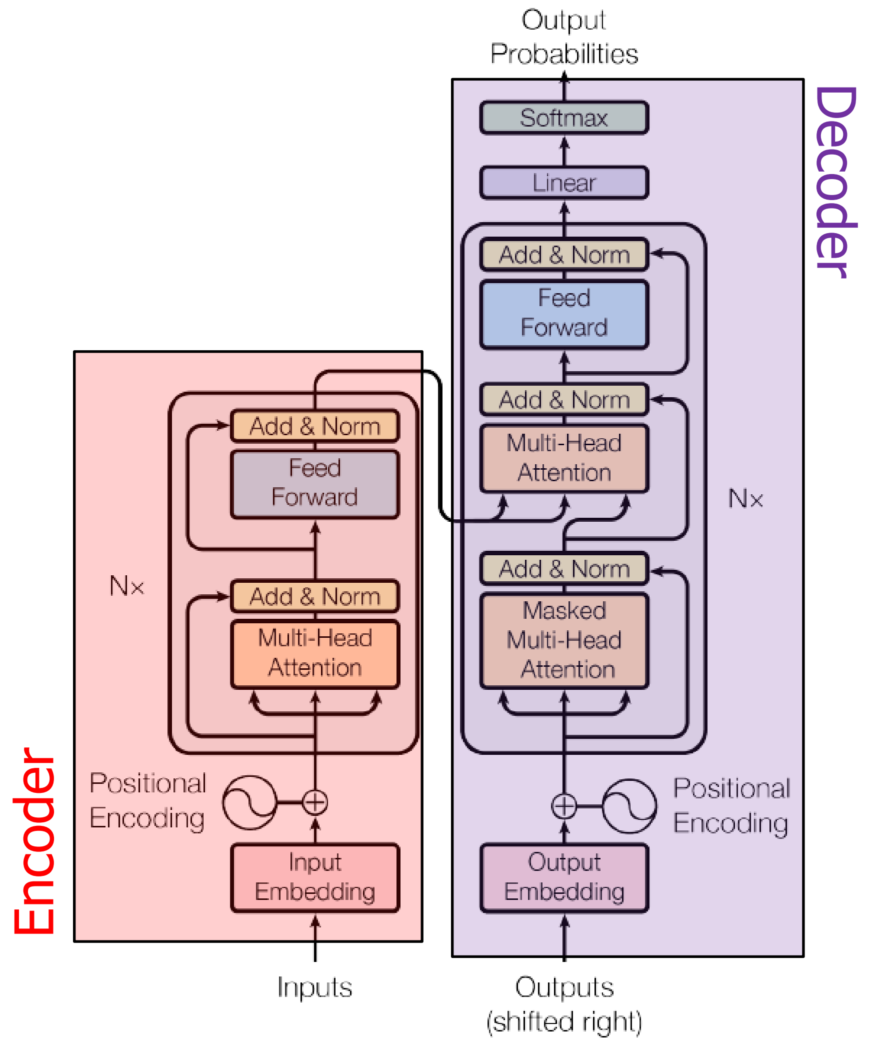
References

BERT Explained: State of the art language model for NLP
Dissecting BERT Part 1: The Encoder
Understanding BERT Part 2: BERT Specifics

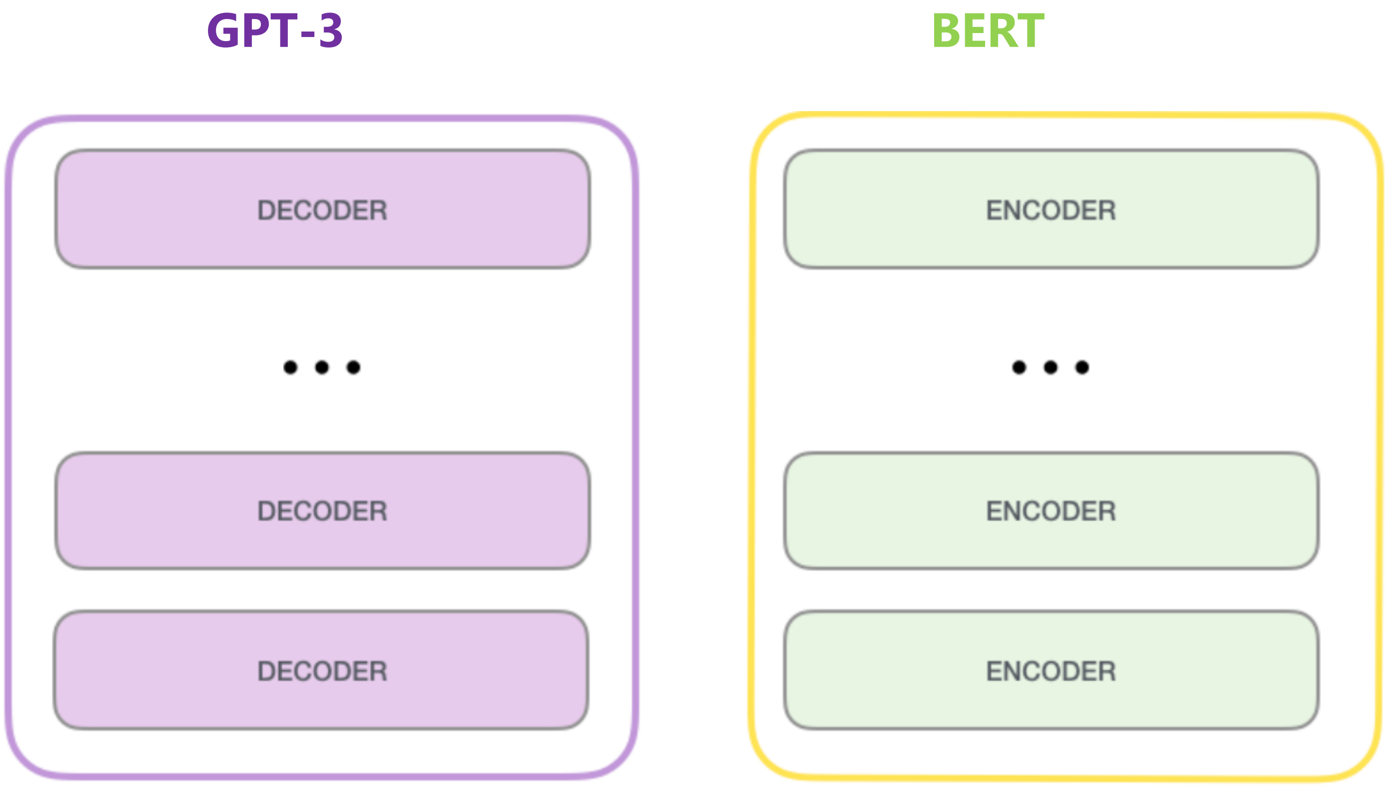
GPT and LLMs

Transformer (Google 2017)

- Transformer was developed for solving text translation problem.
- The Transformer architecture consists of an Encoder and a Decoder and the Encoder's output is an input to the Decoder.



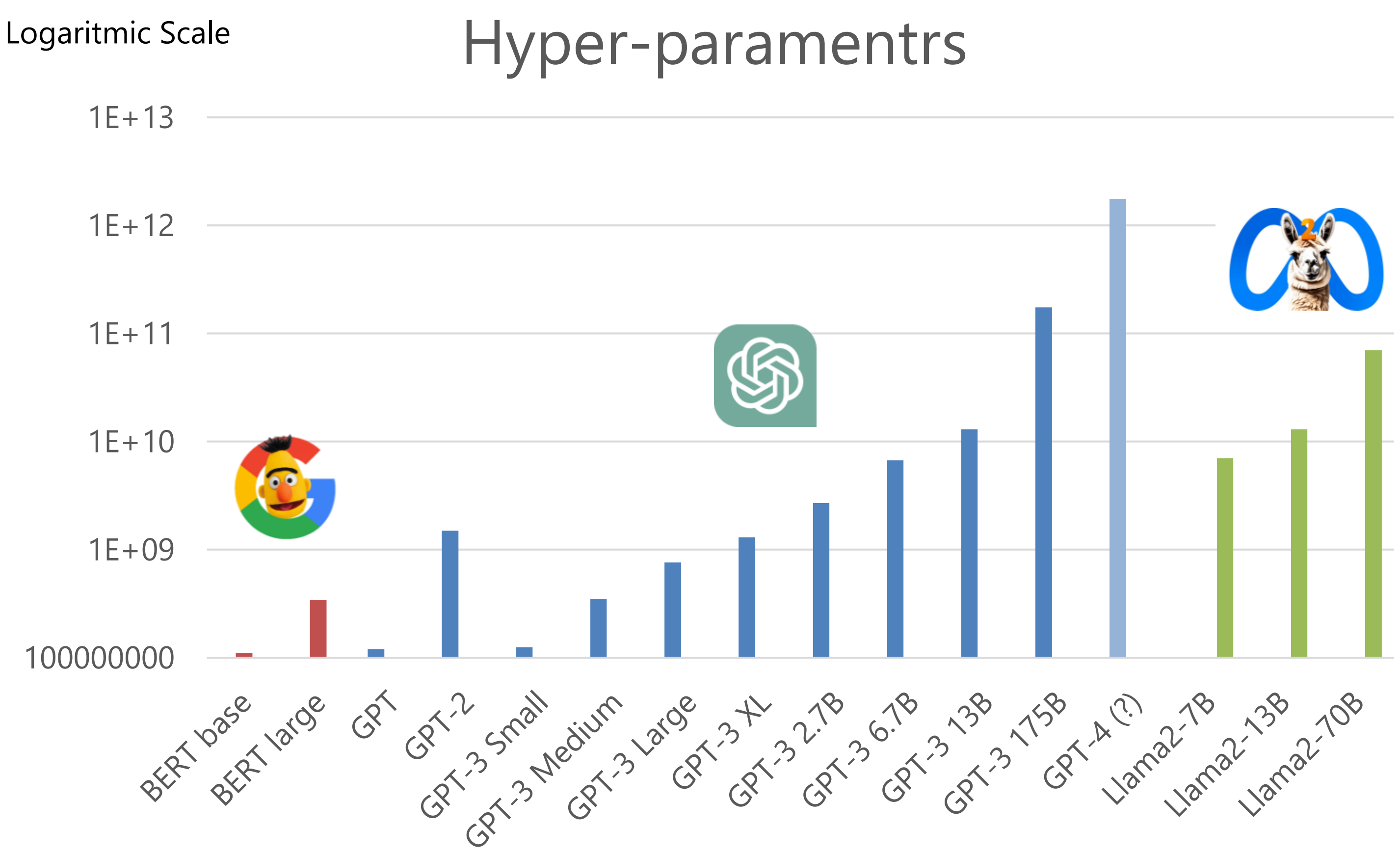
GPT-3 VS BERT


GPT-3
BERT
DECODER
DECODER
DECODER
ENCODER
ENCODER
ENCODER

Hyper-paramentrs

Model Name	n_{params}	n_{layers}	d_{model}	n_{heads}	d_{head}	Batch Size	Learning Rate
GPT-3 Small	125M	12	768	12	64	0.5M	6.0×10^{-4}
GPT-3 Medium	350M	24	1024	16	64	0.5M	3.0×10^{-4}
GPT-3 Large	760M	24	1536	16	96	0.5M	2.5×10^{-4}
GPT-3 XL	1.3B	24	2048	24	128	1M	2.0×10^{-4}
GPT-3 2.7B	2.7B	32	2560	32	80	1M	1.6×10^{-4}
GPT-3 6.7B	6.7B	32	4096	32	128	2M	1.2×10^{-4}
GPT-3 13B	13.0B	40	5140	40	128	2M	1.0×10^{-4}
GPT-3 175B or "GPT-3"	175.0B	96	12288	96	128	3.2M	0.6×10^{-4}

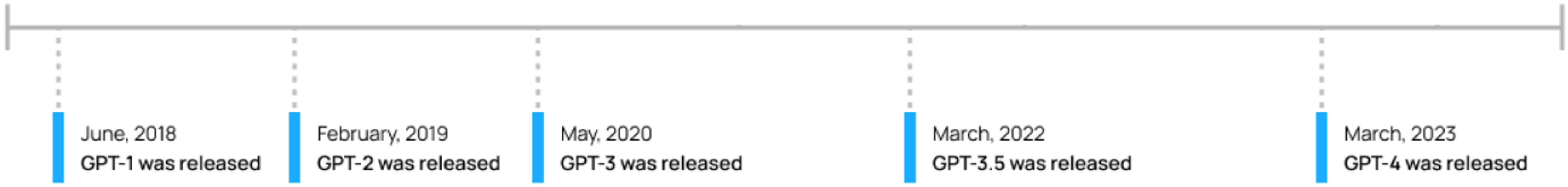
Hyper-paramentrs



Dataset used to Train

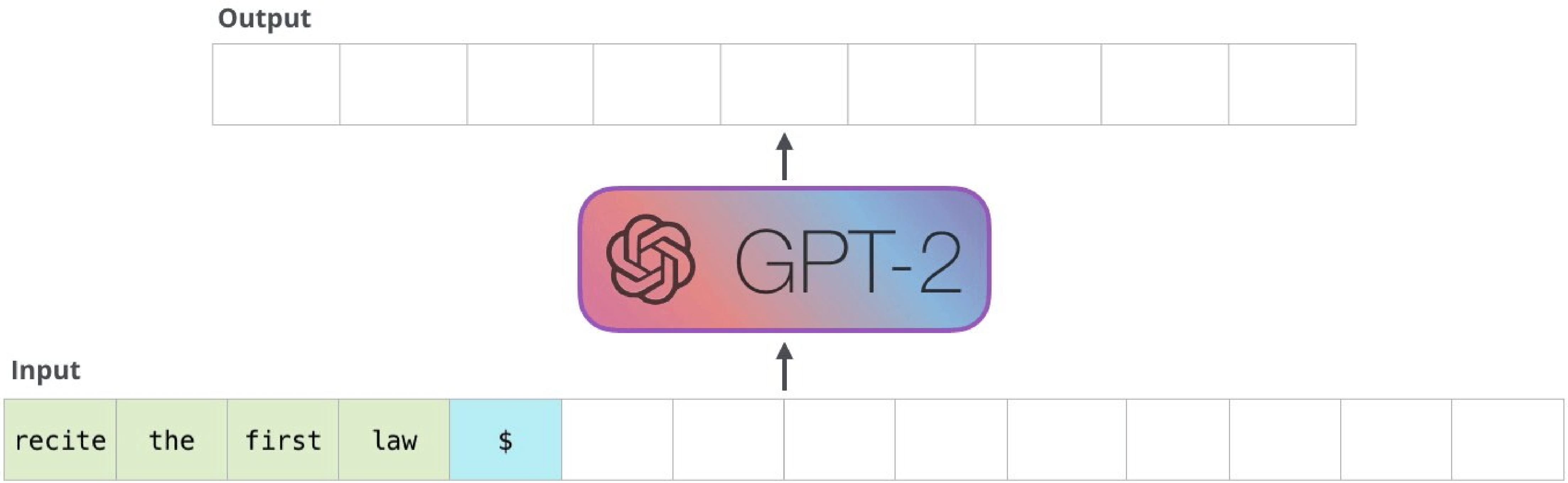
Dataset	Quantity (tokens)	Weight in training mix	Epochs elapsed when training for 300B tokens
Common Crawl (filtered)	410 billion	60%	0.44
WebText2	19 billion	22%	2.9
Books1	12 billion	8%	1.9
Books2	55 billion	8%	0.43
Wikipedia	3 billion	3%	3.4

GPT Family

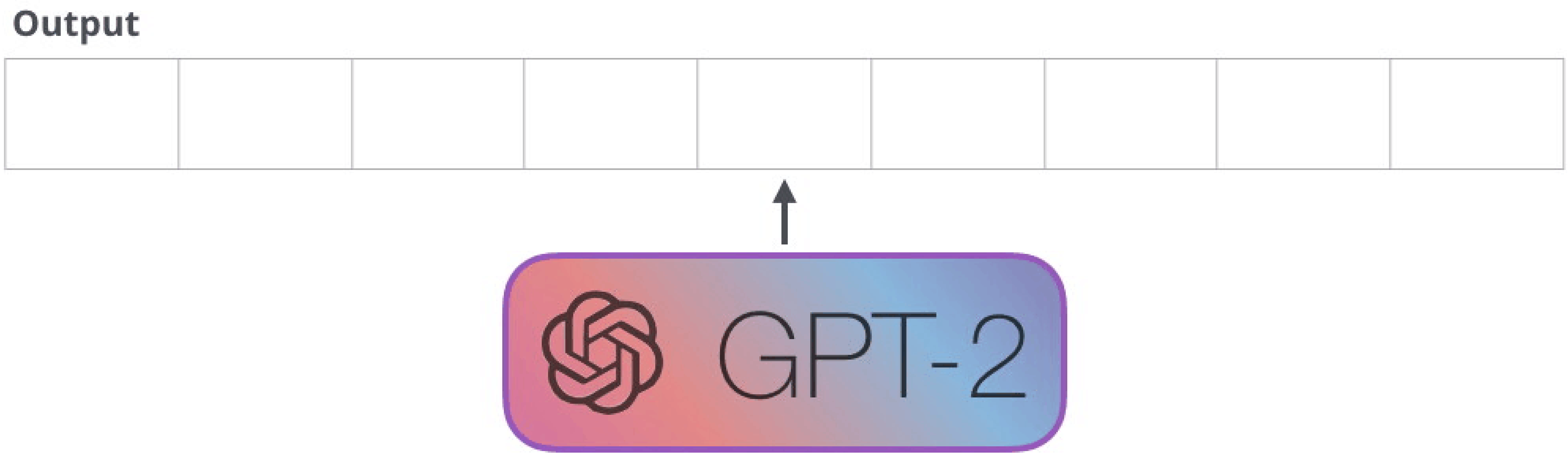

June, 2018
GPT-1 was released
February, 2019
GPT-2 was released
May, 2020
GPT-3 was released
March, 2022
GPT-3.5 was released
March, 2023
GPT-4 was released

Generative Model

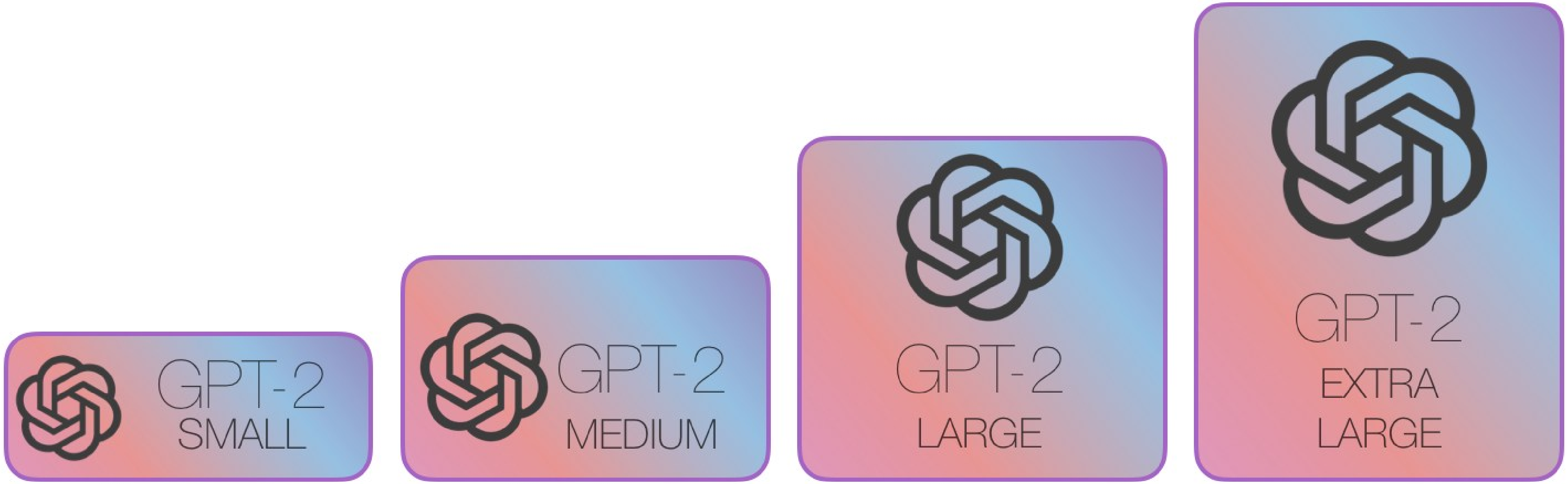
GPT-2 – Difference from BERT



GPT-2

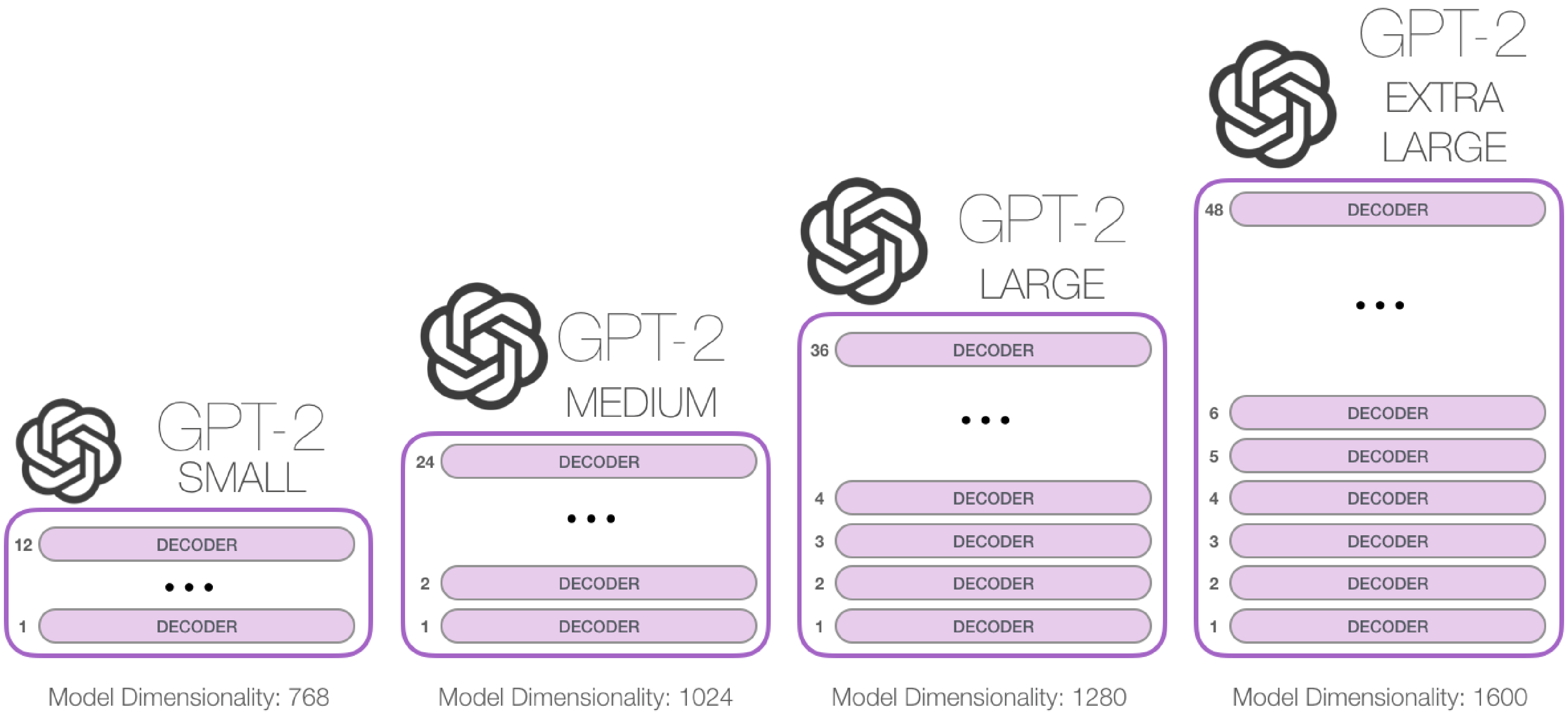


GPT-2



117M Parameters | 345M Parameters | 762M Parameters | 1,542M Parameters

GPT-2

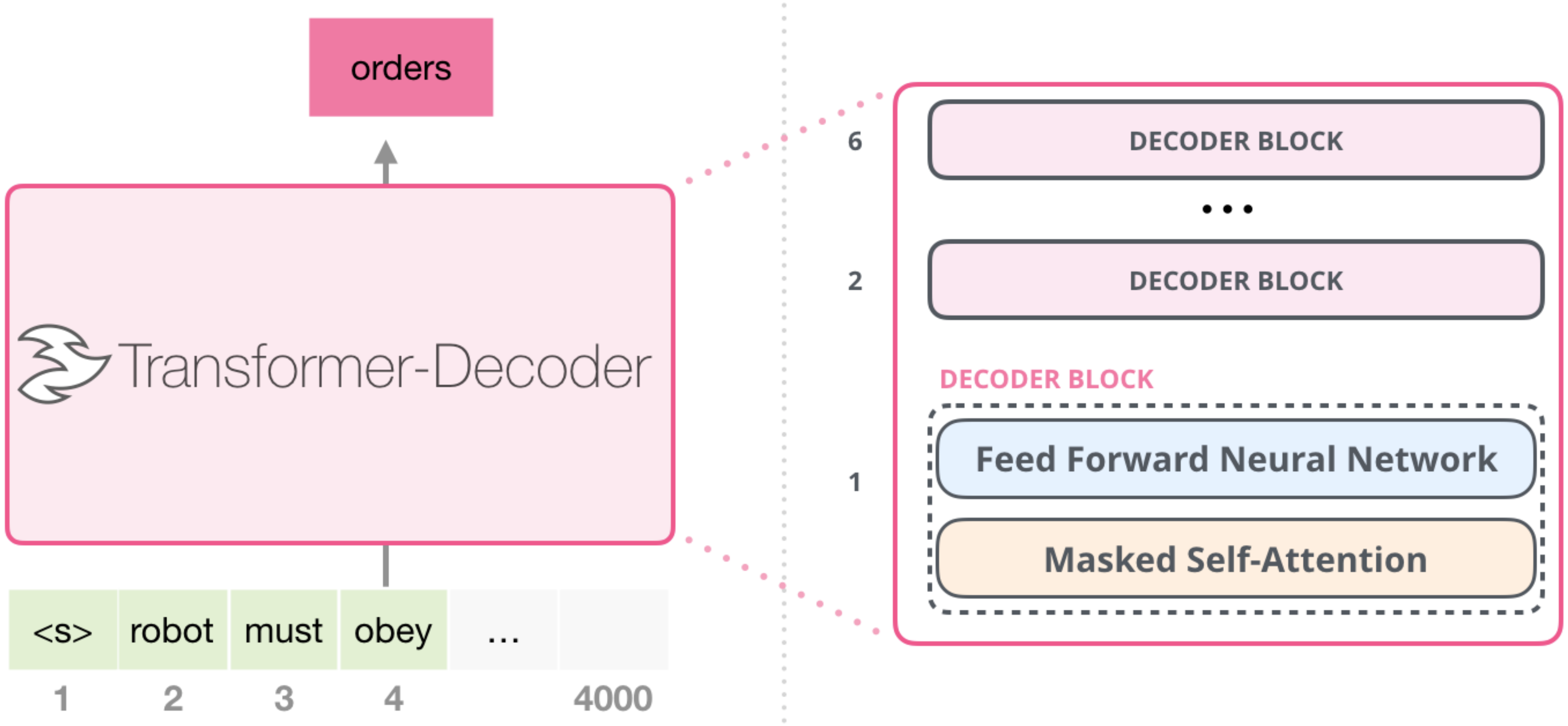

GPT-2
SMALL
12 DECODER
• • •
1 DECODER
Model Dimensionality: 768
GPT-2
MEDIUM
24 DECODER
• • •
2 DECODER
1 DECODER
Model Dimensionality: 1024
GPT-2
LARGE
36 DECODER
• • •
4 DECODER
3 DECODER
2 DECODER
1 DECODER
Model Dimensionality: 1280
GPT-2
EXTRA
LARGE
48 DECODER
• • •
6 DECODER
5 DECODER
4 DECODER
3 DECODER
2 DECODER
1 DECODER
Model Dimensionality: 1600

GPT2 – Key Concept

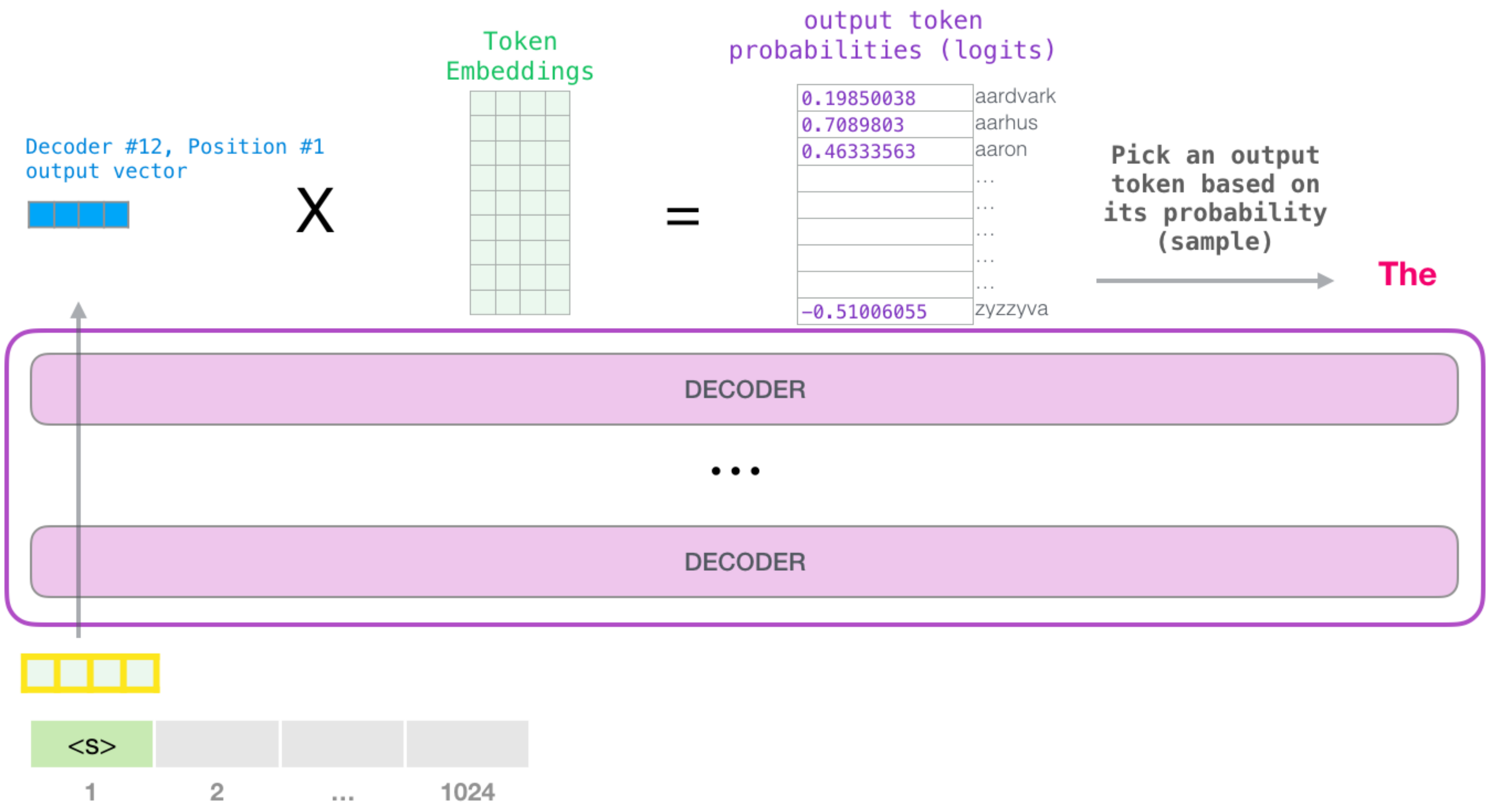
Input Text Sequence:

robot	must	obey	orders
1	2	3	4

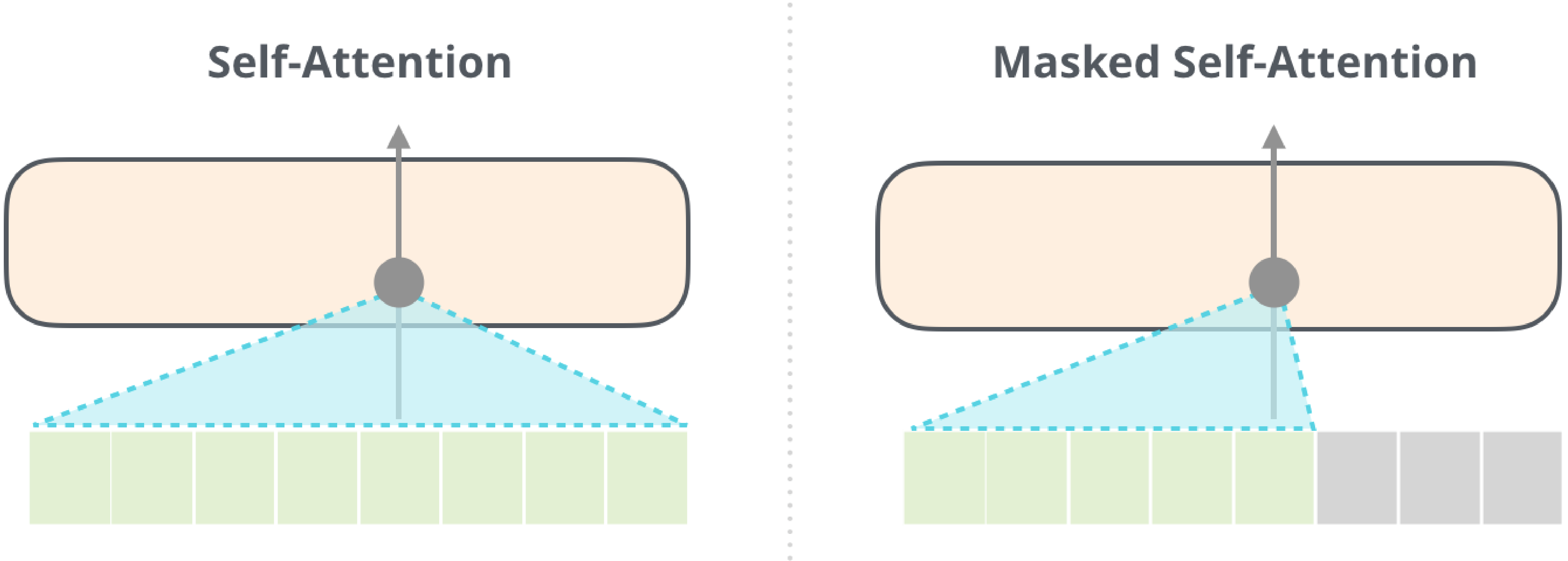
GPT2:



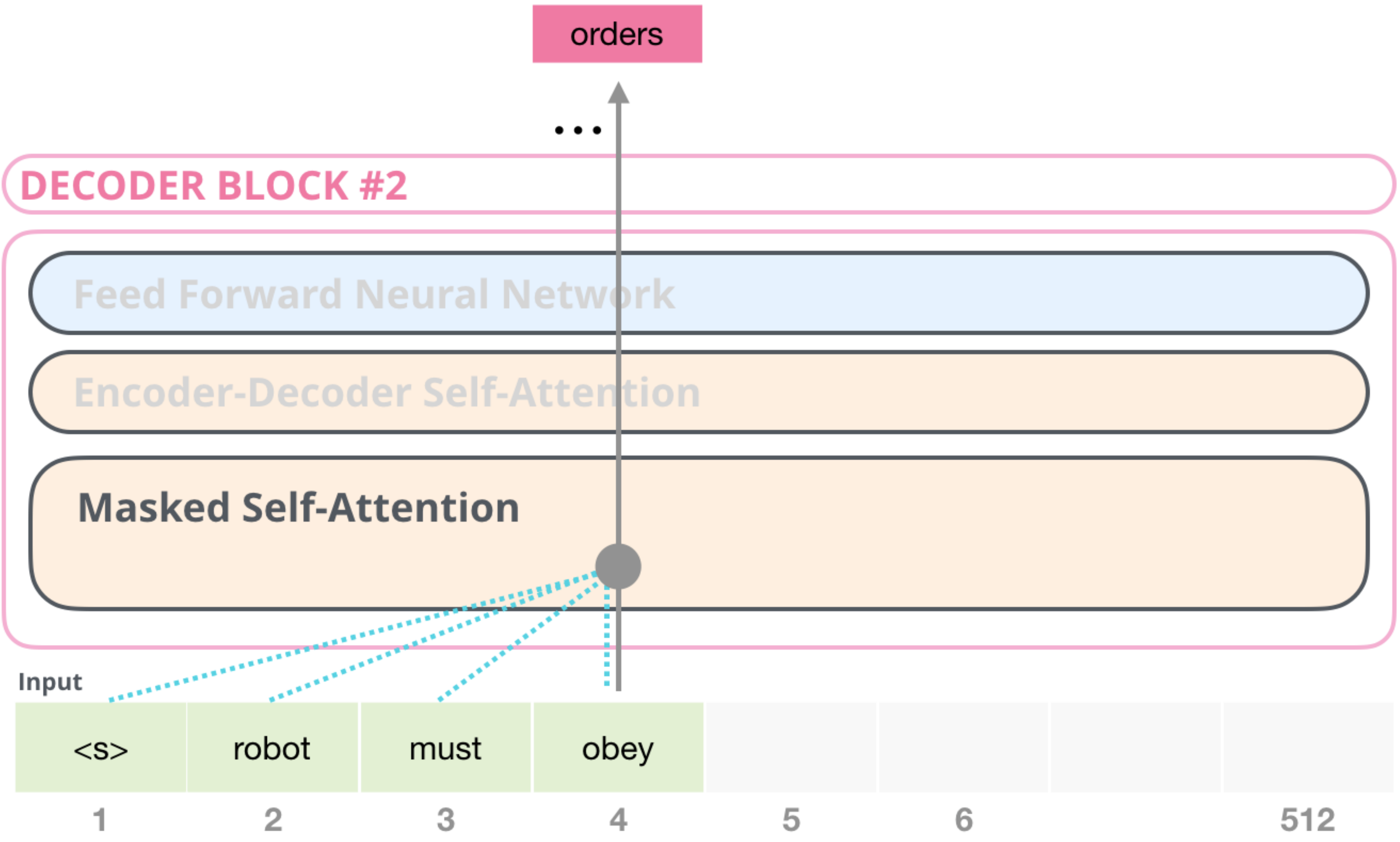
GPT2 – Key Concept



Masked Self-Attention



Masked Self-Attention



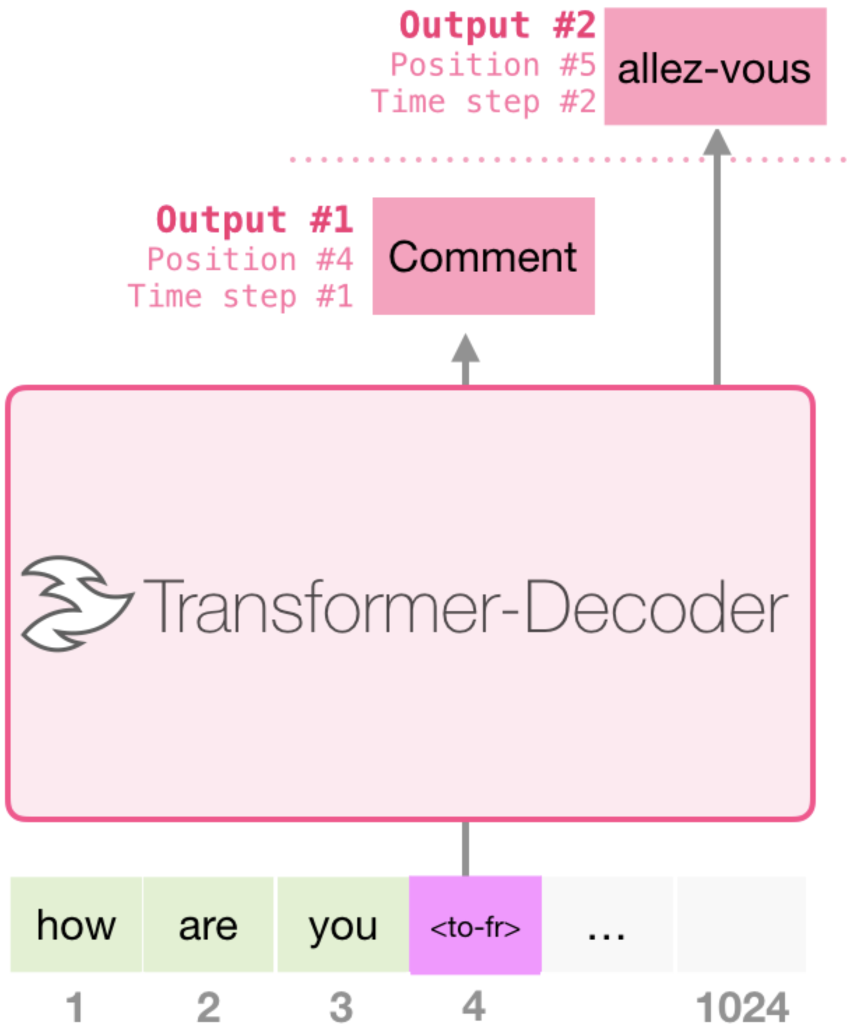
Machine Translation

Video Machine Translation

Machine Translation based on Generative Models

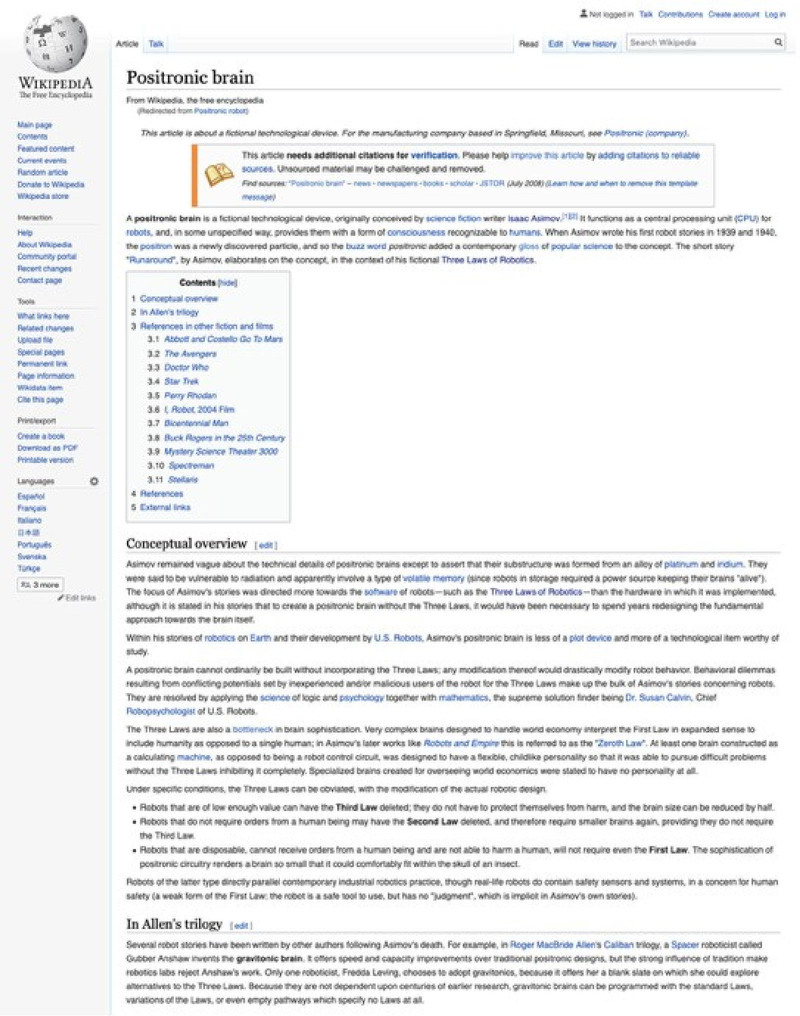
Training Dataset

I	am	a	student	<to-fr>	je	suis	étudiant
let	them	eat	cake	<to-fr>	Qu’ils	mangent	de
good	morning	<to-fr>	Bonjour				



Summarization

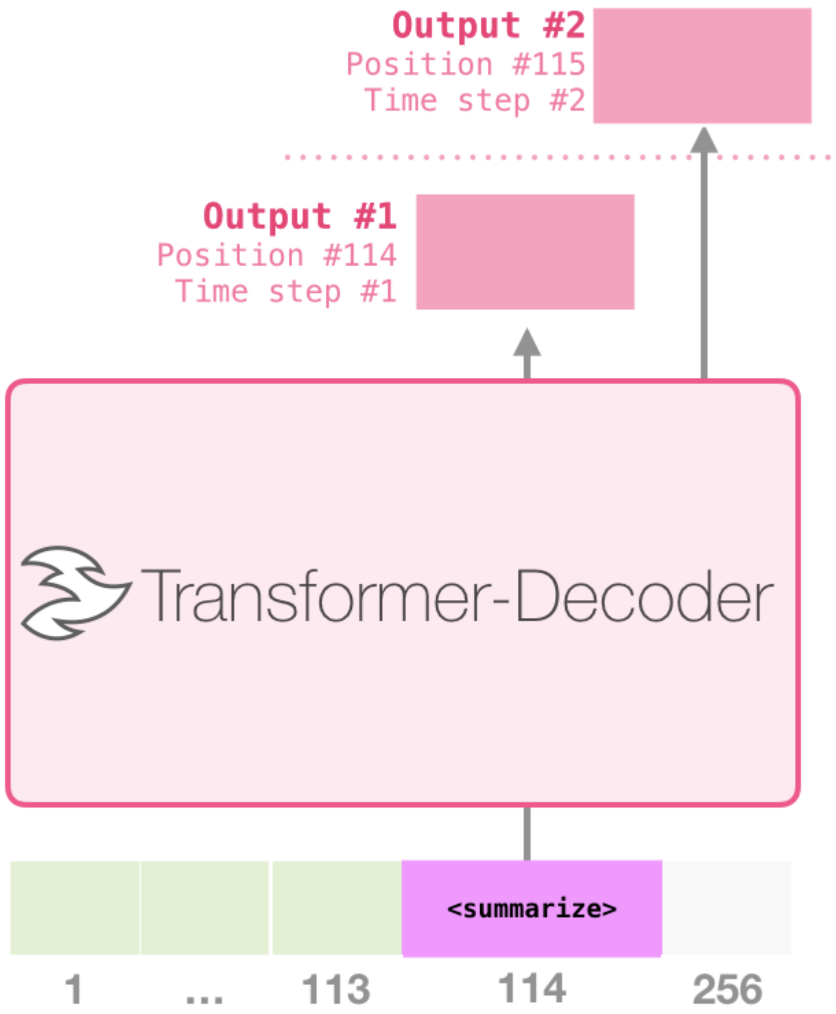
Summarization



GPT2

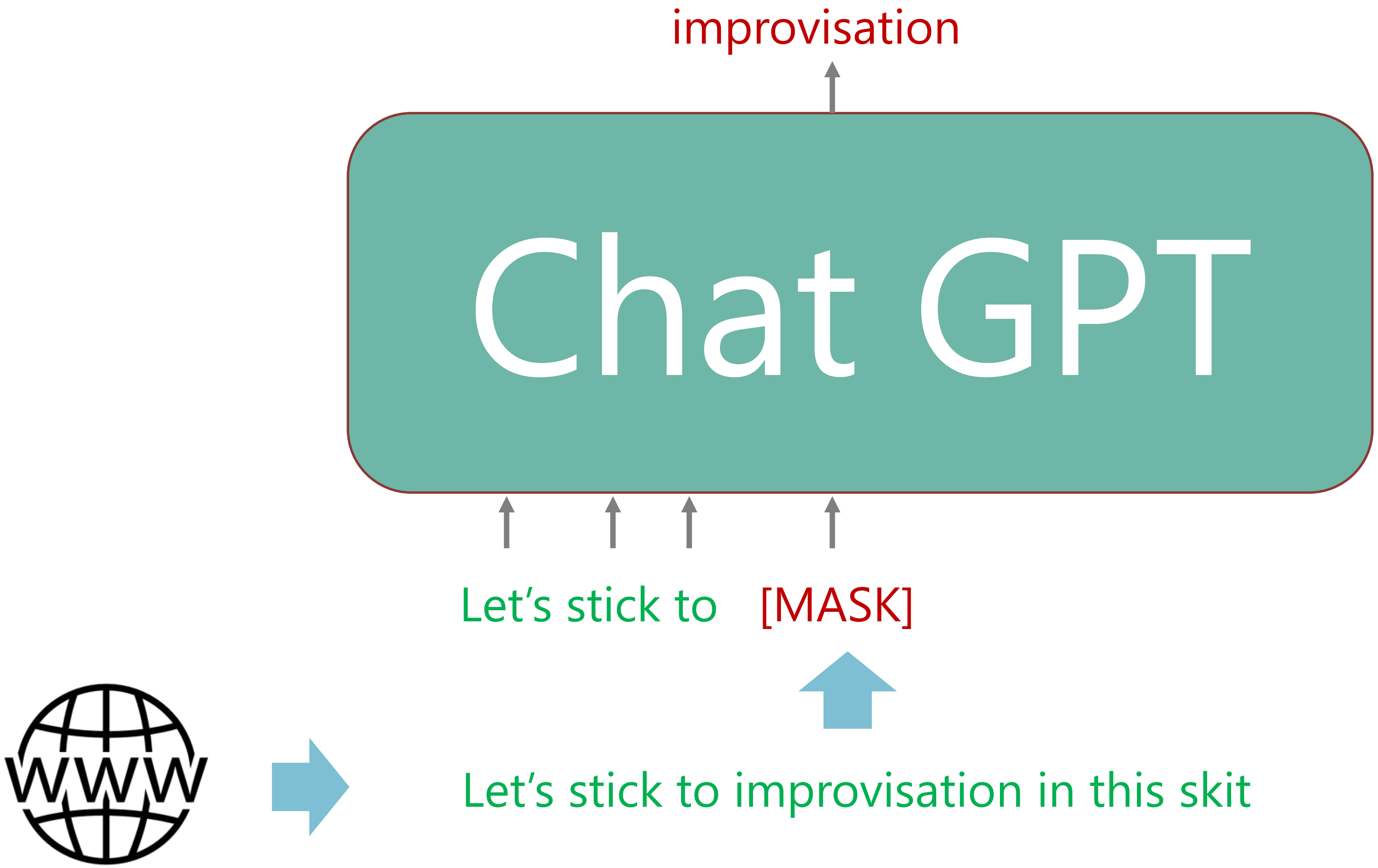
Training Dataset

Article #1 tokens	<summarize>	Article #1 Summary	
Article #2 tokens	<summarize>	Article #2 Summary	padding
Article #3 tokens	<summarize>	Article #3 Summary	

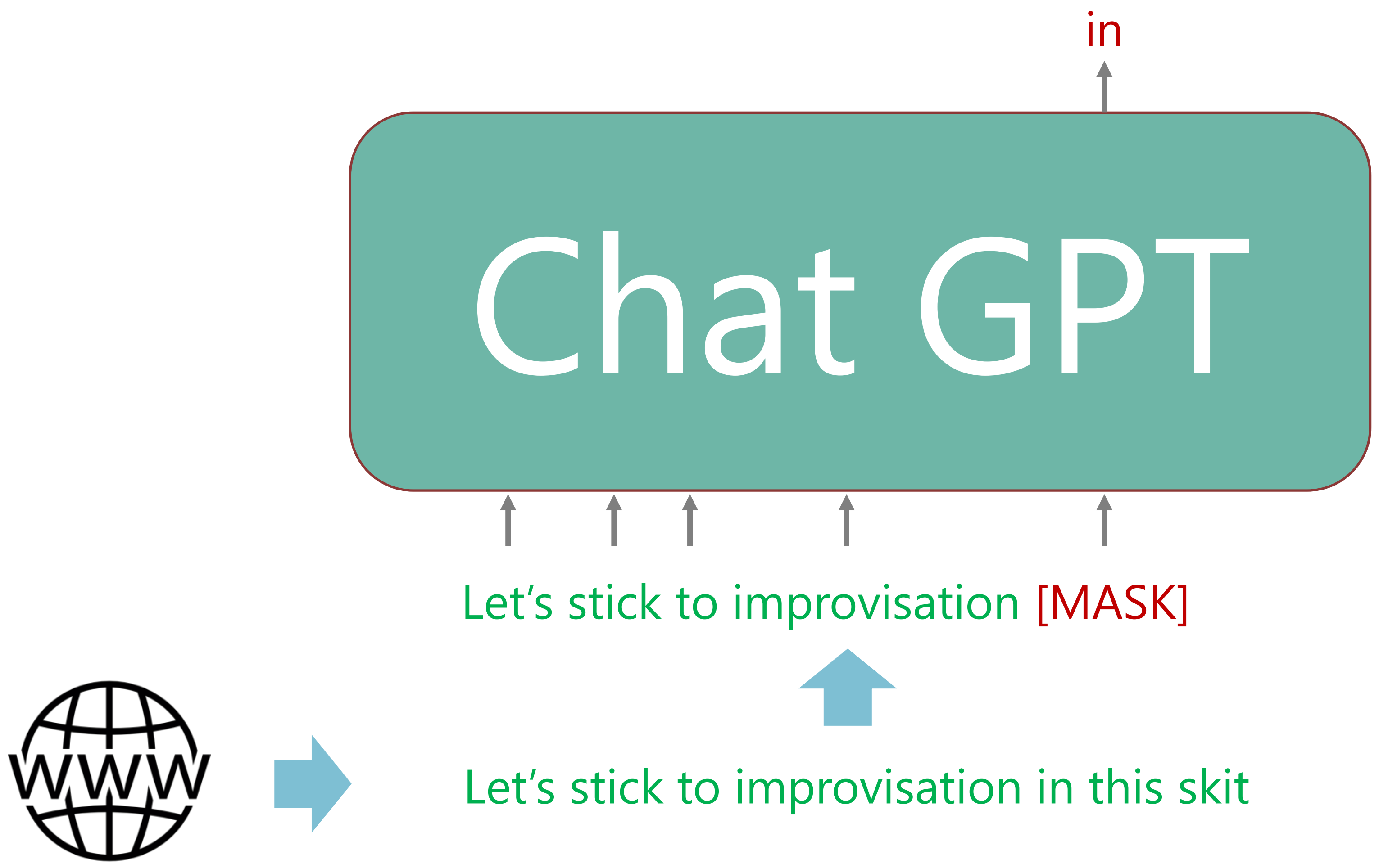


Large Language Models

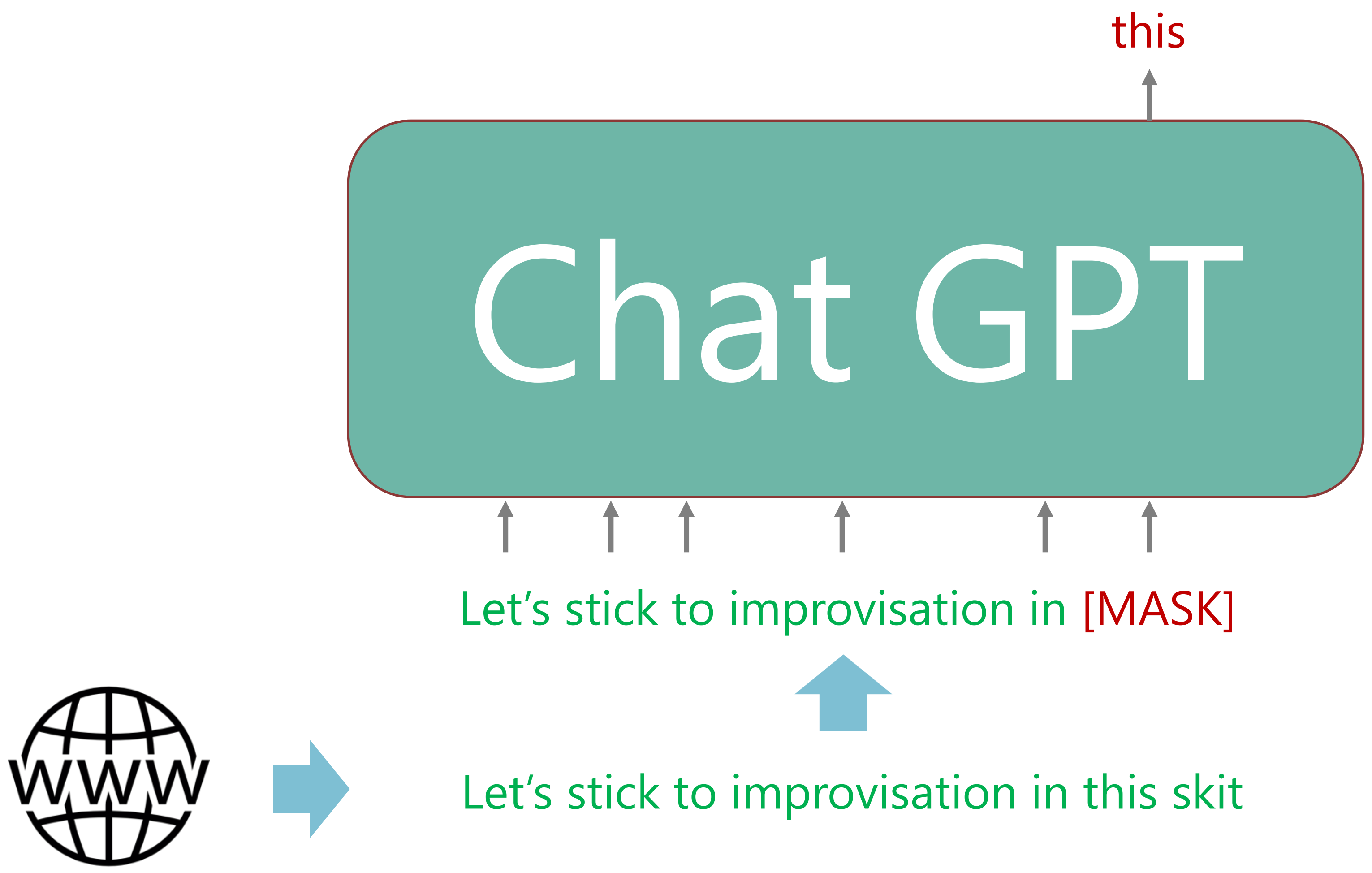
Learning – Step One: Language Model (Self-Supervised Learning)



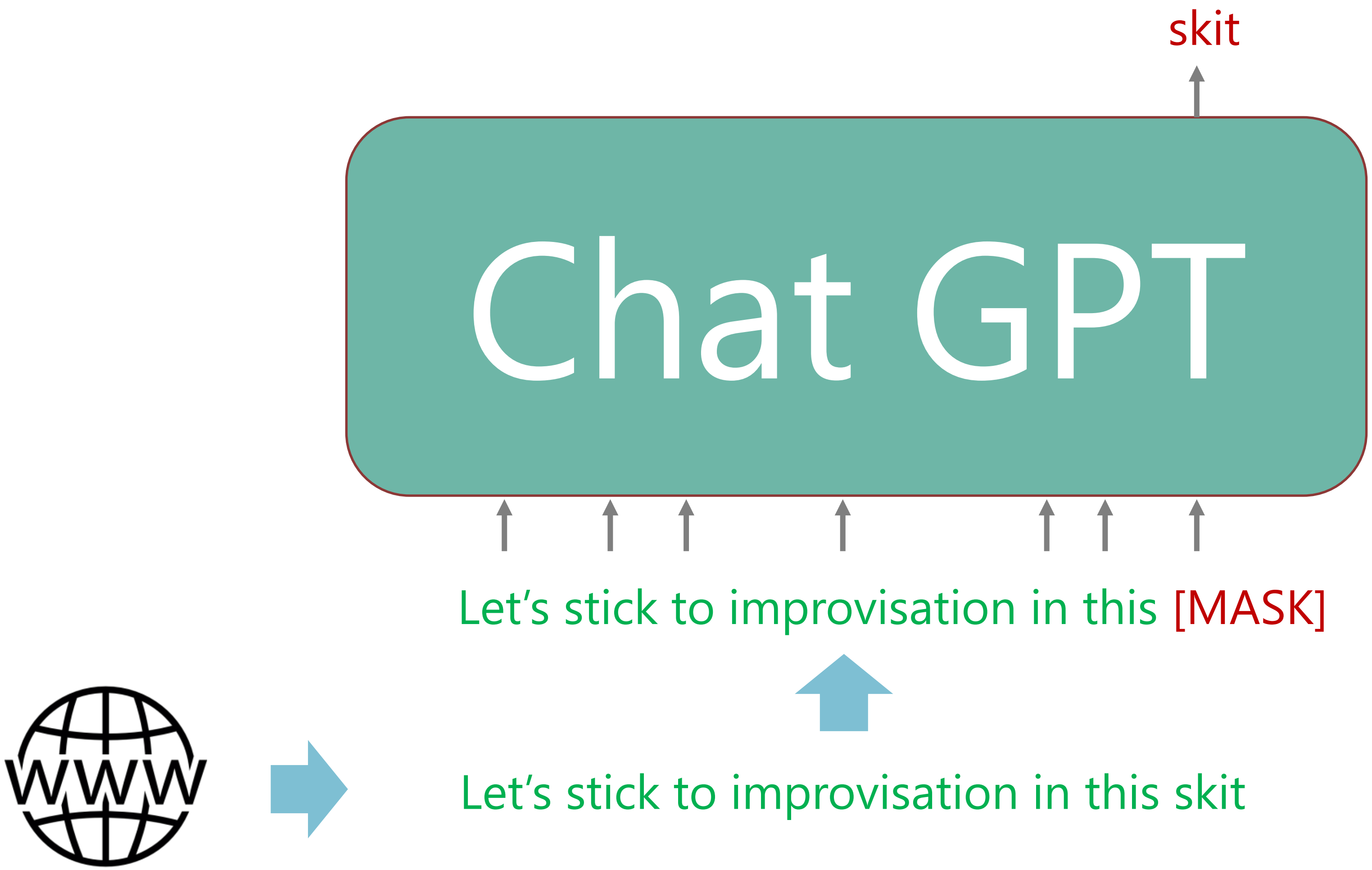
Learning – Step One: Language Model (Self-Supervised Learning)



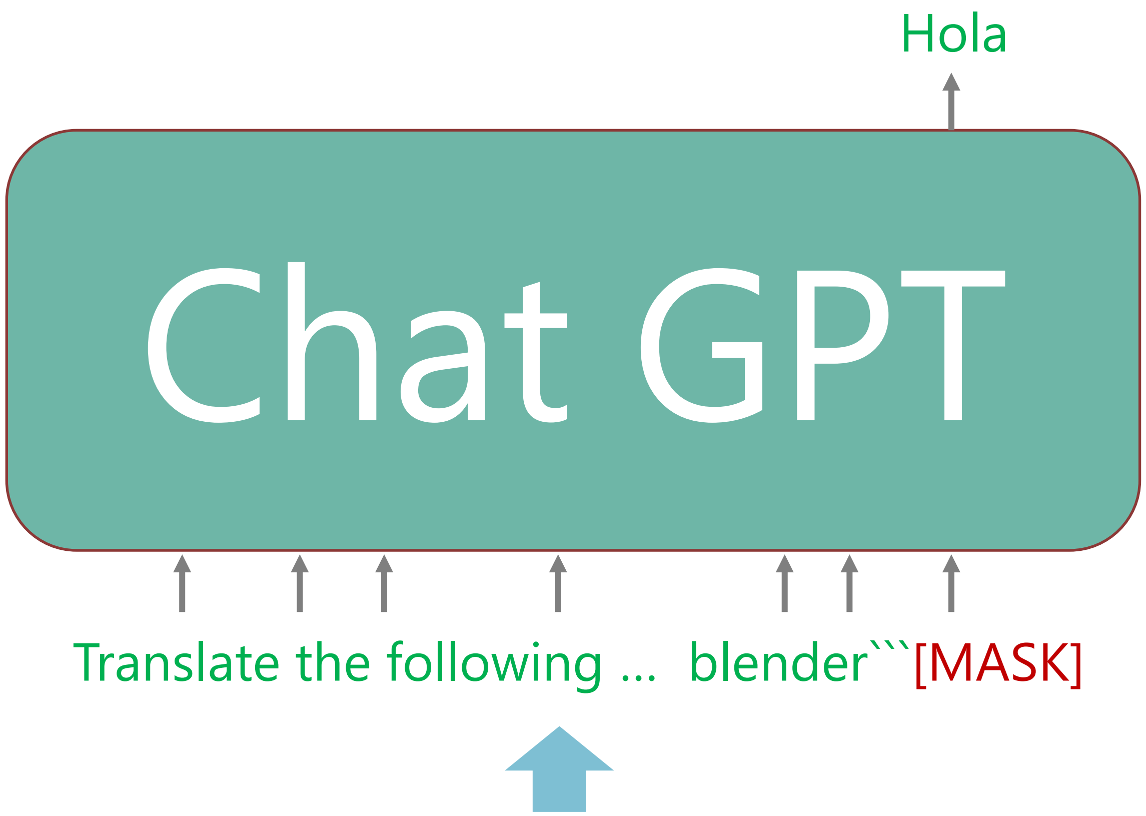
Learning – Step One: Language Model (Self-Supervised Learning)



Learning – Step One: Language Model (Self-Supervised Learning)

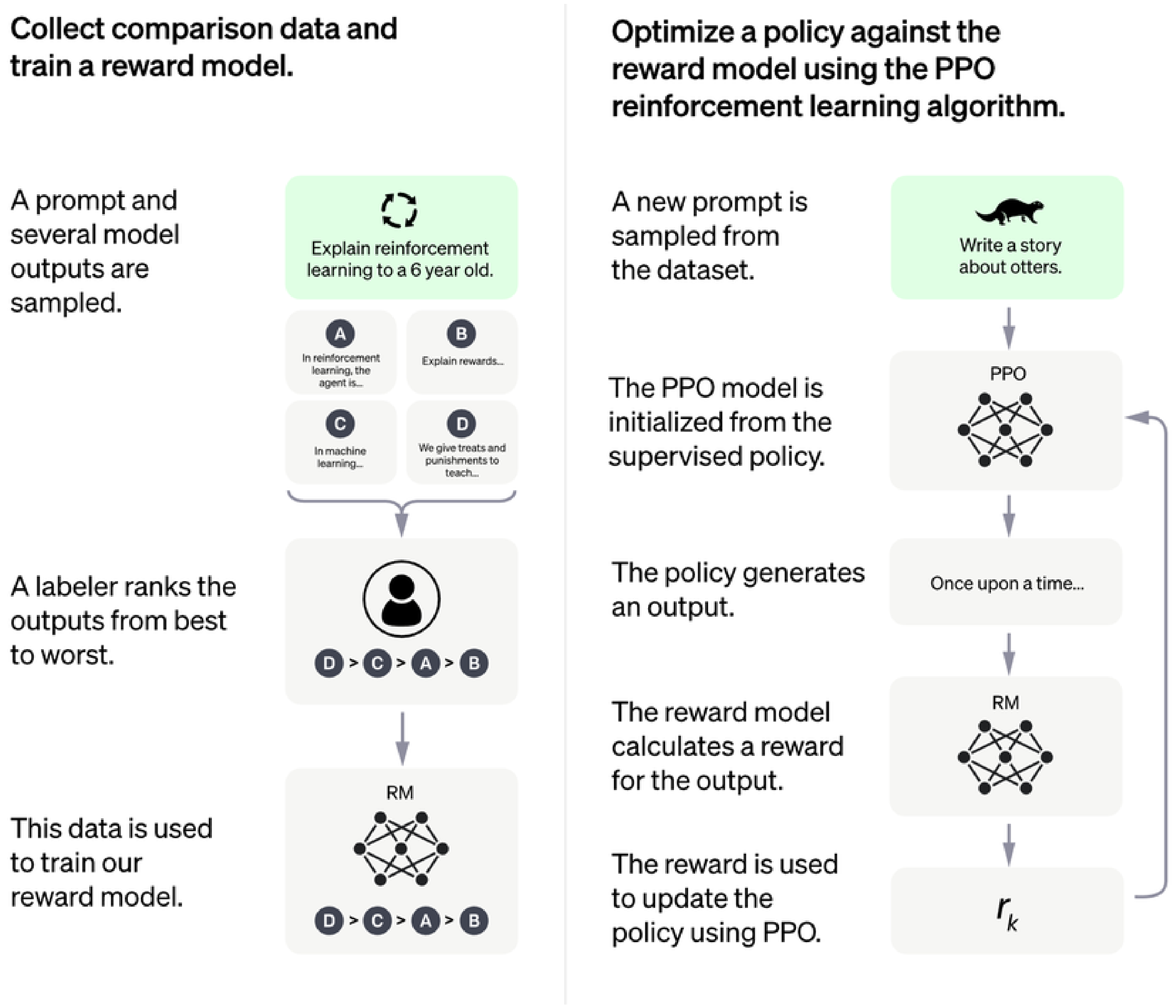


Learning – Step two: Question Answering (Supervised Learning)

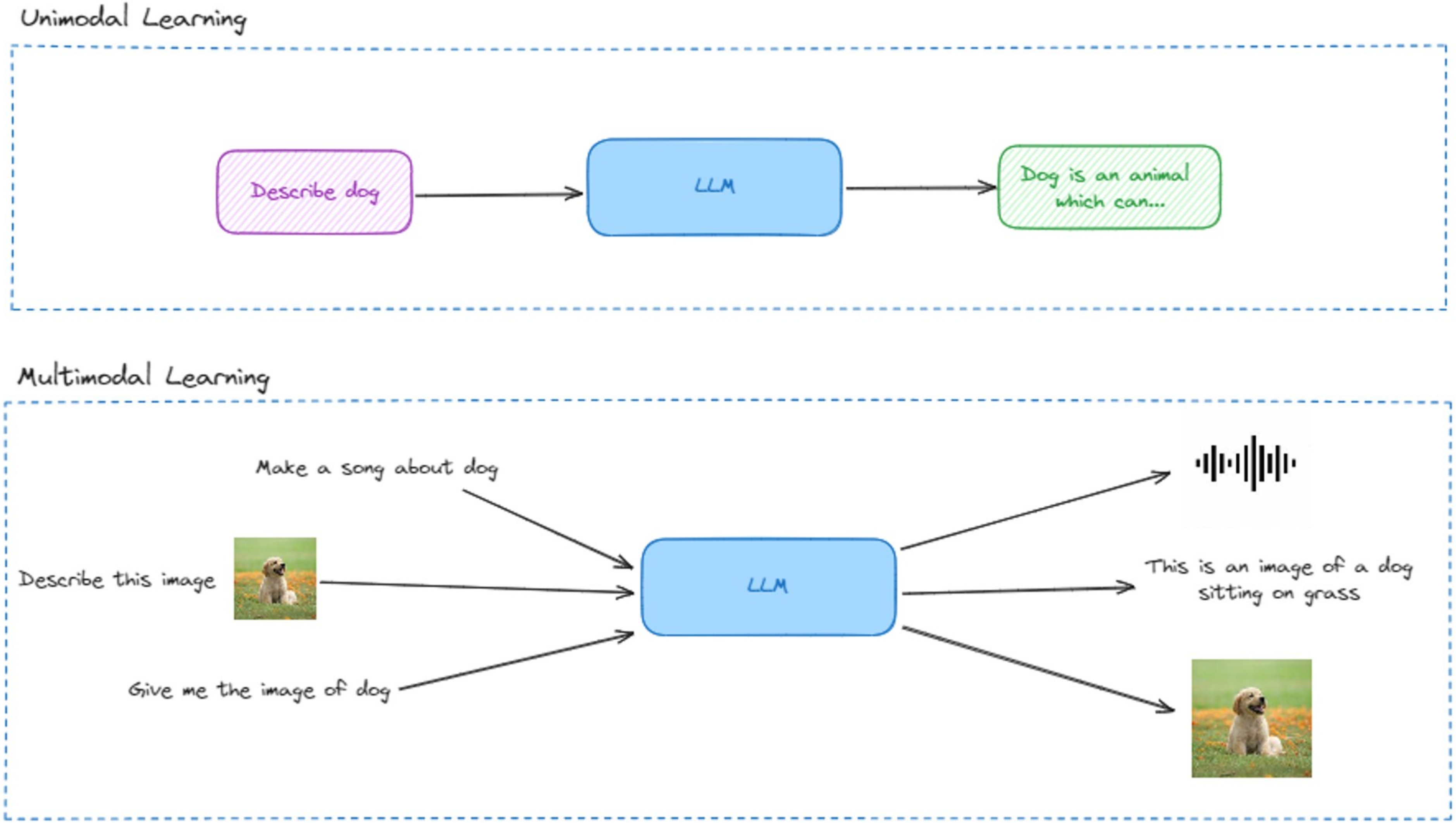


Question: Translate the following English text to Spanish:
```Hi, I would like to order a blender```
Answer: Hola, me gustaría ordenar una licuadora
```

Learning – Step Three: Reinforcement Learning from Human Feedback (RLHF)



MultiModal LLMs

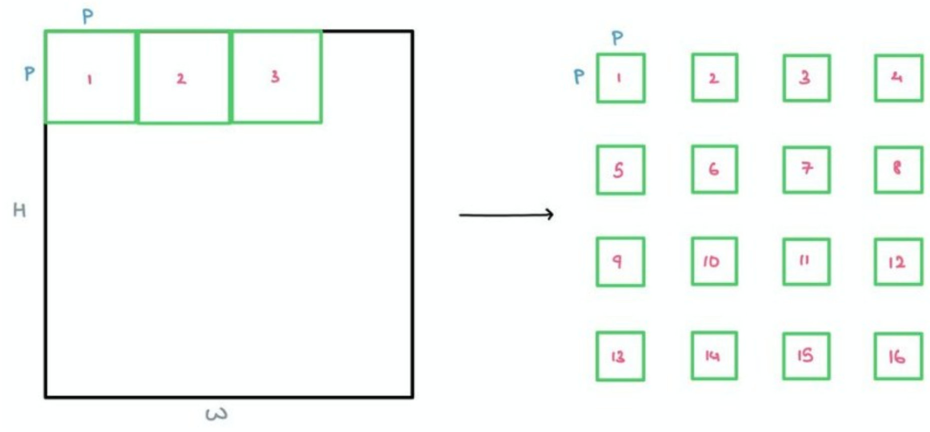


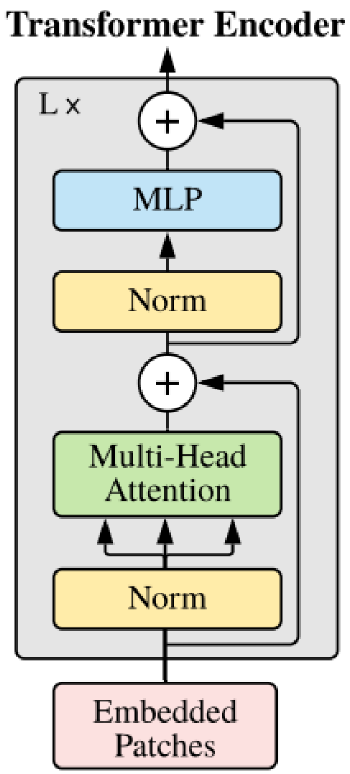
Vision Transformer

Can the mechanism of attention be applied to images?

Yes, Vision Transformer approach (A. Dosovitskiy, 2020), a model based on the transformer encoder used for image processing (classification)

In ViT, the image is "trokenized" into a patch of 16×16 pixels (P×P in general)





MultiModal LLMs